होमी भाभा राष्ट्रीय संस्थान
Homi Bhabha National Institute

शैक्षणिक प्रतिवेदन
Academic Report
2016-17

प्रशिक्षण विद्यालय परिसर
Training School Complex
अणुशक्तिनगर, मुंबई-400 094
Anushaktinagar, Mumbai 400 094

Locations of Constituent Institutions & Off Campus Centre of HBNI

Academic Report 2016-17

Homi Bhabha National Institute

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From the Vice-Chancellor

I am happy to present 2016-2017 annual report of Homi Bhabha National Institute. HBNIwill shortly complete twelve years of its existence. During this period, it has established itself as one of the best research universities in the country encouraging research in various facets of nuclear science and technology including mathematics.

Considering available resources, both in terms of outstanding faculty and vast research infrastructure, HBNI has the potential to expand its academic programmes and introduce innovative programmes including those involving international collaboration. Based on my involvement with the activities of HBNI in last twelve years, I envisage the following three-stage vision plan for HBNI.

Short-Term Vision:

I. To identify areas for research within the mission of the department and break them into doctoral level problems to be taken up by Ph.D. students. Emphasis should be on the areas being projected in the vision document of the department.

II. To vitalize Board of Studies on ‘Applied Systems Analysis’ so that research is undertaken by doctoral students on all topics such as nuclear security, nuclear safeguards, economics of power generation, comparative analysis of various methods of generation of electricity, energy gains of various options of electricity generation, environmental impact, etc. The research should also focus on policy-oriented research into problems of a global nature those are too large or too complex cutting across geographical boundaries of countries.

III. Complete digitization of HBNI central office and its link with all CIs. All students’ and faculty members’ database, including progress monitoring, approval processes and completion documents should be available online.

IV. To encourage students through doctoral committees and board-of-studies to publish more papers in high impact journals. Continue to participate in NAAC accreditation and NIRF yearly ranking processes or any other similar statutory requirements decided by Govermnment of India.

V. To convert HBNI into an Institute of National Importance: HBNI has several unique characteristics. All these characteristics do not lend them to governance by the same system as a conventional university and flexibility offered by the INI status is necessary.

Medium-Term Vision:

I. To ramp up intake to doctoral programme in BARC to 125 students per year. This is in addition to employees pursuing the Ph.D. programme. This will amount to starting a parallel training school program in BARC.

II. To include other units of DAE such as NFC, AMD, new campuses of TMC and IPR, etc. under the ambit of HBNI academically.

III. To start PG medical programmes at all departments of TMC and BARC Hospital and to start integrated MD-PhD programme in TMC.

IV. Provisions to start research projects by HBNI. To invite foreign nationals from premier institutions from India/abroad as visiting faculty members and researchers.

V. To continue to assess areas needing research to meet the target set by the DAE and divide all such areas into doctoral level problems to be addressed by doctoral students.

Long-Term vision:

I. To align academic programmes with the National programmes; National Technology Mission, National Skill Mission, Make in India etc. To provide an academic environment which will promote innovation, creativity and breakthrough research in the multidisciplinary areas.

II. To raise the status of the HBNI such that it is unquestionably recognized as a world class Research University.

Finally, I may say that the previous year was a very rewarding year. HBNI will continue to provide an academic environment which will promote innovation, creativity and breakthrough research in the multidisciplinary areas aligning with the mandate of the department. Above vision plan may provide us a firm direction to raise its status so that it is recognized as a world class Research University with a significant global ranking.

BK Dutta

(B.K.Dutta)

Introduction

The HBNI has the following as its Constituent Institutions (CIs)/ Off Campus Centre (OCC)

1. Bhabha Atomic Research Centre (BARC), Mumbai
2. Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam
3. Raja Ramanna Centre for Advanced Technology (RRCAT), Indore
4. Variable Energy Cyclotron Centre (VECC), Kolkata
5. Saha Institute of Nuclear Physics (SINP), Kolkata
6. Institute for Plasma Research (IPR), Gandhinagar
7. Institute of Physics (IOP), Bhubaneswar
8. Harish-Chandra Research Institute (HRI), Allahabad
9. Institute of Mathematical Sciences (IMSc), Chennai, and
10. Tata Memorial Centre (TMC), Mumbai.
11. National Institute of Science Education and Research (NISER), Bhubaneswar (from February 5, 2016)

The role of HBNI is to nurture in-depth capabilities in nuclear science and engineering and to serve as a catalyst to accelerate the pace of basic research and facilitate its translation into technology development and applications through academic programs, viz., Master's and Ph.D. degrees in Engineering, Physical, Chemical, Mathematical, Life and Health Sciences while encouraging inter-disciplinary research. Additionally, a Strategic Studies program has also been identified to ensure availability of adequate qualified human resources to address issues pertaining to nuclear law, economics of nuclear power, nuclear security, nuclear proliferation, intellectual property rights etc.

In 2006, the Government of India decided to strengthen science education and set up institutions for science education and research in various parts of the country. One such institution, the National Institute for Science Education and Research (NISER) was setup at Bhubaneswar by the Department of Atomic Energy (DAE) as a project of the Institute of Physics. Academic programs of this institute were started as a part of IOP and thereby under HBNI. MHRD declared NISER an off campus centre (OCC) of HBNI vide notification no. F.10-3/2011-U.3(A) dated Feb 5, 2016.

Academic Programs of the Institute

The HBNI offers a range of academic programs in chemical sciences, engineering sciences, health sciences, life sciences, mathematical sciences and physical sciences. It also has a program in strategic studies. All institutions, except NISER, conduct programs at post-graduate level. Various programs offered are the following.

Ph.D. in varied disciplines is offered at all CIs. HRI and IMSc also offer an integrated Ph.D. program where students study for M.Sc. as well as Ph.D. NISER has proposed to start similar Ph.D. program.

M.Tech. in engineering sciences and **M.Phil.** in physical sciences, chemical sciences and life sciences. These programs consist of one year of course work and one year of project work. The course work is offered at all campuses of BARC Training School and IPR Training School. Project work is offered at BARC, IGCAR, RRCAT, VECC, IPR and some other units of DAE. Those who are not interested in project work get a post graduate diploma in lieu of M.Tech. or M.Phil degree.

M.Sc. (Engg) in which research content is more than that in a M.Tech. program. The duration of the project work under this program is one and half year, while the duration of the course work is up to one year. This program is offered at BARC, IGCAR, VECC, RRCAT and IPR.

Integrated M.Sc.of five-year duration at NISER

Super Specialty Health Science Courses at TMC

- **D.M.** (Medical Oncology)
- **D.M.** (Pediatric Oncology)
- **D.M.** (Gastroenterology)
- **D.M.** (Critical Care Medicine)
- **D.M.** (Interventional Radiology)
- **M. Ch.** (Surgical Oncology)
- **M. Ch.** (Gynecological Oncology)
- **M.Ch.** (Plastic Surgery)
- **M.Ch.** (Head & Neck Oncology)

Post Graduate Health Science Courses at TMC

- **M.D.** (Pathology)
- **M.D.** (Anesthesia)
- **M.D.** (Radio-diagnosis)
- **M.D.** (Radiotherapy)
- **M.D.**(Microbiology)
- **M.D.**(Nuclear Medicine)
- **M.D.** (Palliative Medicine)
- **M.D.** (Immuno-Hematology &Blood Transfusion)

DRM: Diploma in Radiation Medicine at BARC.
M.Sc. (Nursing)atTMC
M.Sc. (Clinical Research)atTMC
Dip.R.P.: Diploma in Radiological Physics at BARC
DMRIT: Diploma in Medical Radio Isotope Techniques at BARC.
PGDFIT: PGDiploma in Fusion Imaging Technology at TMC

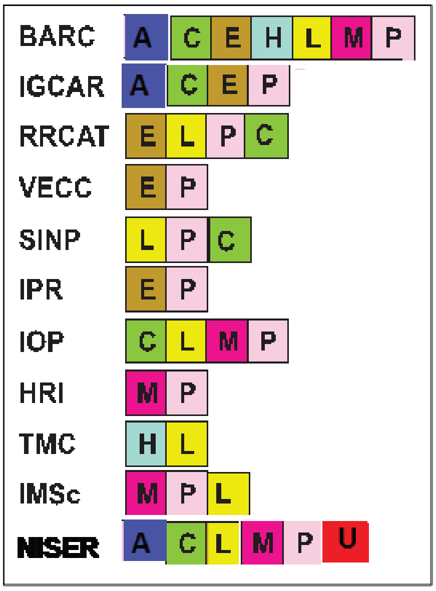
In addition, the TMC also offers a two-year Certified Fellowship Program in 23 different areas related to Oncology.Most of the Ph.D. programsare multi-disciplinary in nature having guides and co-guides from different branches of science and engineering.Nine hundred and fourteen students are admitted in different programs during 2016-17, out of which 353 students are for PhD program. HBNI has awarded 218 Ph.D., 106M.Tech., 10 M.Sc. (Engg), 73 M.Sc., 107 post graduate medical degrees, 6 M.Sc.(Nursing) and 42PG diplomas in radiation protection (DipRP),medical radioisotope technology (DMRIT), radiation medicine (DRM) and fusion imaging technology (DFIT) during this period.All the Constituent Institutions have excellent library facilities having a large collection of books and subscribe to a large number of research journals. All journals are available to researchers on their desktops.

Composition of the Bodies of the Institute

Management of the Institute

The Council of Management is the principal organ for the management of the Institute. All academic issues are handled by an Academic Council which functions on the advice of the Board of Studies. There is a Board of Studies for every discipline as follows.

- Applied systems analysis (A)
- Chemical Sciences (C)
- Engineering Sciences (E)
- Health Sciences (H)
- Life Sciences (L)
- Mathematical Sciences (M)
- Physical Sciences (P)
- Undergraduate Studies (U)



BARC	A	C	E	H	L	M	P
IGCAR	A	C	E	P			
RRCAT	E	L	P	C			
VECC	E	P					
SINP	L	P	C				
IPR	E	P					
IOP	C	L	M	P			
HRI	M	P					
TMC	H	L					
IMSc	M	P	L				
NISER	A	C	L	M	P	U	

To manage the affairs of the Institute at the level of Constituent Institutions (CIs), each CI has one or more Deans-Academic and a university cell. CIs have also established a robust framework for admission, evaluation of performance and monitoring the progress of research by the students.

Advisory Committee

Chairman, AEC	Chairman	Director, TMC	Member
Vice Chancellor, HBNI	Member	Director, IMSc	Member
Director, BARC	Member	Director, TIFR	Member
Director, IGCAR	Member	Director, NISER	Member
Director, RRCAT	Member	Director, HRI	Member
Director, VECC	Member	Director, IoP	Member
Director, IPR	Member	Dean, HBNI	Member-Secretary
Director, SINP	Member		

Officers of the Institute

Academic

Prof. B.K. Dutta	Vice Chancellor (Officiating) (w.e.f. 01/03/2016)
Prof. P.D. Gupta	Vice Chancellor (From 14/09/16)
Prof. B.K. Dutta	Dean
Prof. D. K. Maity	Associate Dean
Prof. A.K. Dureja	Associate Dean

Administrative and Accounts

Shri Himanshu Shankar	Finance Officer
Dr. Avichal Kapur	Registrar (Up to 31/12/2016)
Prof. B.K. Dutta	Registrar (Officiating, w.e.f. 01/01/2017)
Shri M.S. Gandle	Deputy Registrar
Shri T. Nagendran	Finance Officer
Ms. B. Lata	Administrative Officer
Ms. Bharati Suverna	Asst.Registrar

Board of Studies of HBNI (As on 31st of March 2017)

BoS (Physical Sciences)

1. Prof. A. K. Mohanty

2.Prof. G. Amarendra

3.Prof. Sudip Sengupta

4.Prof. Shikha Varma

5.Prof. S. B. Roy

6.Prof. Pinaki Majumdar

7.Prof. D. Indumathi

8.Prof. S. R. Banerjee

9.Prof. N. K. Sahoo

10.Prof. S. C. Gadkari

Balancing Members:

1.Prof. B. S. Tomar

2.Prof. G. K. Dey

BoS (Chemical Sciences)

1.Prof. B. S. Tomar

2.Prof. D. K. Maity

3.Prof. P. K. Pujari

4.Prof. S. Anthony Samy

5.Prof. A. Srinivasan

6.Prof. S. Kannan

7.Prof. H. Pal

8.Prof. A. K. Tyagi

9.Prof. P. D. Naik

10.Prof. M. Saibaba

Balancing Members:

1.Prof. A. K. Mohanty

2.Prof. S. Chattopadhyay

3. Prof. (Mrs.) S. Banerjee

BoS (Life Sciences)

1.Prof. S. Chattopadhyay

2.Prof. B. J. Rao

3.Prof. Abhijit Chakraborty

4.Prof. (Mrs.) S. Chiplunkar

5.Prof. Rajiv Sarin

6.Prof. S. Gautam

7.Prof. S. Santoshkumar

8.Prof. H. S. Mishra

9.Prof. P. Suprasanna

Balancing Members:

1.Prof. K. S. Sharma

2.Prof. B. S. Tomar

BoS (Engineering Sciences)

1.Prof. G. K. Dey

2.Prof. G. Sasikala

3.Prof. A. P. Tiwari

4.Prof. K. Velusamy

5.Prof. Archana Sharma

6.Prof. P. V. Varde

7.Prof. D. N. Badodkar

8.Prof. A. K. Nayak

9.Prof. J. Chattopadhyay

10.Prof. S. Mukherjee

Balancing Members:

1.Prof. A. K. Mohanty

2.Prof. B. S. Tomar

BoS (Mathematical Sciences)

1.Prof. B. Ramakrishnan

2.Prof. Meena Mahajan

3.Prof. R. R. Puri

4.Prof. Punita Batra

5.Prof. Mahuya Datta

6.Prof. Jugal K. Verma

7.Prof. K. V. Subrahmanyam

8.Prof. V. Muruganandam

9.Prof. B. Sury

10.Prof. K. N. Raghavan

BoS (Health Sciences)

1. Prof. K. S. Sharma

2. Prof. N. Roy

3. Prof. Nalini Shah

4. Prof. Suleman Merchant

5. Dr. S. K. Srivastava

6. Dr. S. V. Kane

7. Dr. S. B. Banavali

8. Prof. P. S. Yadav

9. Prof. Sandeep Basu

10. Prof. D. D. Deshpande

Balancing Members:

1. Prof. S. V.Chiplunkar

2. Prof. S. Chattopadhyay

BoS (Applied Systems Analysis)

1.Prof. R. B. Grover

2.Dr. K. Raghuraman

3.Prof. M. Sai Baba

4.Prof. P. D. Gupta

5.Prof. G. Ravikumar

6.Dr. Pranay Swain

7.Dr. C.S. Pramesh

8.Prof. Surinder Jaswal

BoS (Undergraduate Studies)

1.Prof. V. Chandrashekhar

2.Dr. Bedangadas Mohanty

3.Dr. Anil Karn

4.Dr. Chandan Goswami

5.Prof. A. Srinivasan

6.Dr. Pranay Swain

7.Dr. Harapriya Mohapatra

8.Dr. Joydeep Bhattacharya

Balancing Members:

1.Prof. Pinaki Majumdar

2.Prof. D. K. Maity

3.Prof. Meena Mahajan

4.Prof. S. Chattopadhyay

Deans Academic at Constituent Institutions (CIs)/Off-Campus Centre

S. No.	Name of CI/Off-Campus Centre	Discipline	Name of Dean Academic
1.	Bhabha Atomic Research Centre (BARC), Mumbai	Engineering Sciences	Prof. G K Dey
		Chemical Sciences	Prof. A. K. Tyagi
		Physical & Mathematical Sciences	Prof. Saibal Basu
		Health Sciences	Prof. Sandip Basu
		Life Sciences	Prof. Hema Rajaram
2.	Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam	Chemical Sciences	Prof. S Anthonysamy
		Physical Sciences	Prof. N V Chandra Shekar
		Engineering Sciences	Prof. G. Sasikala
3.	Raja Ramanna Centre for Advanced Technology (RRCAT), Indore		Prof. Arup Banerjee
4.	Variable Energy Cyclotron Centre (VECC), Kolkata	Physical Sciences	Prof. Jane Alam
		Engineering Sciences	Prof. Paramita Mukherjee
5.	Saha Institute of Nuclear Physics (SINP), Kolkata	Physical Sciences	Prof. Debades Bandyopadhyay
		Chemical and Life Sciences	Prof. Abhijit Chakrabarti
6.	Institute for Plasma Research (IPR), Gandhinagar		Prof. S Mukherjee
7.	Institute of Physics (IoP), Bhubaneswar		Prof. Pankaj Agrawal
8.	Harish-Chandra Research Institute (HRI), Allahabad		Prof. B. Ramakrishna
9.	Tata Memorial Centre (TMC), Mumbai		Prof. K S Sharma
10.	Institute of Mathematical Science (IMSc.), Chennai	Mathematical Sciences	Prof. Vijay Kodiyalam
		Physical Sciences	Prof. Purusattam Ray
		Life Sciences	Prof. Gautam Menon
11.	National Institute for Science Education and Research (NISER), Bhubaneswar		Prof. Harapriya Mohapatra

Faculty List (As on January 1st, 2017)

BARC

❖ Chemical Sciences

1 Achary S. N.
2 Acharya Raghunath
3 Adhikari Soumyakanti
4 Agarwal Renu
5 Alamelu D.
6 Arya Ashok Kumar
7 Awadhesh Kumar
8 Bandyopadhyay Tusar
9 Banerjee Aparna
10 Banerjee Sharmila
11 Bhardwaj Y. K.
12 Bhasikuttan A C
13 Bindal R. C.
14 Chandrakumar K R S
15 Chatterjee Suchandra
16 Chattopadhyay Subrata
17 Choudhury Niharendu
18 Das Smruti
19 Das Tapas
20 Dash Ashutosh
21 Deo Mukul Narayan
22 Dey Ghasiram
23 Dey Sandip
24 Dhanya S
25 Dubey Abhinav Kumar
26 Dutt G. B.
27 Dutta Choudhury Sharmistha
28 Dutta Dimple
29 Ganguly R
30 Ghanty Tapan Kumar
31 Ghosh Asim Kumar
32 Ghosh Hirendra Nath
33 Ghosh Subir Kumar
34 Ghosh Sunil Kumar
35 Ghosh Swapan K
36 Goswami Madhumita
37 Gupta Vinita Grover
38 Hassan P A
39 Jain V K
40 Jha Shambhu Nath
41 K Indira Priyadarsini
42 Kadam Ramakant Mahadeo
43 Kapoor Sudhir
44 Kaushik Chetan Prakash
45 Kedarnath G.
46 Korde Aruna
47 Kshirsagar R J
48 Kumar Pradeep
49 Kumar Sangita D.
50 Kumar Sanjiv
51 Kumar Sanjukta A.
52 Kumar Sunil Jai
53 Kumar Virendra
54 Maity Dilip Kumar
55 Majumder Chiranjib
56 Manmohan Kumar
57 Mishra Adya Prasad
58 Mishra R
59 Misra N L
60 Mohanty J.
61 Mohapatra Prasanta Kumar
62 Mukerjee S K
63 Murali M. S.
64 Musharaf Ali S. K.
65 Naik Devidas B
66 Naik Prakash Dattatray
67 Naik Yeshwant Padmakar
68 Nath Sukhendu
69 Nayak A. K.
70 Nayak Sandip Kumar
71 Ningthougam Raghumani Singh
72 Pabby Anil Kumar
73 Pai Mrinal R.
74 Pal Haridas
75 Palit Dipak Kumar
76 Pandey Ashok Kumar
77 Pandey Usha
78 Pandit Gauri Girish
79 Parida Suresh Chandra
80 Patra Chandra Nath
81 Pujari Pradeep Kumar
82 R. Sasikala
83 Raje Naina
84 Ramkumar Jayshree

85 Rangarajan S
86 Rath M.C.
87 Ravi P. M.
88 Ray Alok Kumar
89 Roy Mainak
90 Sabharwal Sunil
91 Sali S. K.
92 Samanta Alok Kumar
93 Sarkar S K
94 Satpati Ashis Kumar
95 Sawant Shilpa N.
96 Sharma Anubha
97 Sharma Pramod
98 Shashikala K.
99 Singh Ajay K
100 Singh Kumar Dhurva
101 Singhal Anshu
102 Singhal Rakesh Kumar
103 Sodaye Hemant Shivram
104 Sodaye Suparna
105 Sreenivas T
106 Srinivasan M. P
107 Srivastava Ritu M.
108 Sudarsan V.
109 Sudarshan Kathi
110 Sunny Febby
111 Tomar B S
112 Tripathi A. K.
113 Tripathi R M
114 Tyagi A K
115 Upadhyaya Hari Prasad
116 Varshney Lalit
117 Vatsa R K
118 Velmurugan S
119 Venkatesh Meera
120 Banerjee Dayamoy
121 Bhattacharya Arunasis
122 Kumbhakar Manoj
123 Kunwar Amit
124 Mondal Jahur A
125 Phadnis Prasad
126 Rao Ankita
127 Rufus A L
128 Sarkar Arnab
129 Satpati Drishty
130 Swain K. K.

❖ Engineering Sciences

131 Awasthi Alok
132 Badodkar D N
133 Balasubramaniam R
134 Banerjee S.
135 Betty C A
136 Bhargava Kapilesh
137 Bhattacharjee Anup Kumar
138 Biswas Aniruddha
139 Chakraborty Sankar Prasad
140 Chakraborty Sudipta
141 Chakravarty Anindya
142 Chattopadhyay Jayanta
143 Chaturvedi Shashank
144 Das Ramkrishna
145 Dey Gautam Kumar
146 Dikshit Biswaranjan
147 Dutta B K
148 Dwarakanath T A
149 Gopalakrishnan Sugilal
150 Gopika Vinod
151 Grover Ravi Bhushan
152 Kain Vivekanand
153 Kapoor Rajeev
154 Kar D C
155 Khan Imran Ali
156 Khan Kirity Bhushan
157 Laik Arijit
158 Mahata Tarasankar
159 Maheshwari N K
160 Mandal D.
161 Mukhopadhyaya Sulekha
162 Nayak Arun Kumar
163 Pal Sangita
164 Patankar V H
165 Prakash Deep
166 Reddy G R
167 Roy Debanik
168 Roy Kallol
169 Roy S B (Mrs.)
170 Samal M K
171 Sengupta Pranesh
172 Sharma Archana

173 Singh Gursharan
174 Singh Jung Bahadur
175 Singh K. K.
176 Singh R K
177 Singh Ram Niwas
178 Srivastava Dinesh
179 Taliyan S S
180 Tewari P K
181 Tewari Raghvendra
182 Tiwari A P
183 Topkar Anita Vinay
184 Tripathy Prabhat Kumar
185 U Saravana Kumar
186 Varde Prabhakar V
187 Vincent Tessy
188 Vinod Kumar A
189 Vijayan P K
190 Chandraker Dinesh Kumar
191 Dureja Adarsh Kumar
192 Kar Soumitra
193 Mukhopadhyay Siddharatha
194 Sinha Amit
195 Vaidya Abhijeet Mohan
196 Verma Rishi

❖ Health Sciences

197 Basu Sandip
198 Gadgil Anita (Ms.)
199 Jadhav D. S.
200 Jadhav R. V.
201 Kalbhande
202 Khandekar A. J. (Ms.)
203 Kulkarni A. R. (Ms.)
204 Malhotra Gaurav
205 Malpani B. L.
206 Mishra Satish
207 More N. N. (Ms.)
208 Pendse R. R.
209 Roy N.
210 Saha Swapnil
211 Sharma Sunil Dutt
212 Shejul Yogesh K
213 Tamboli Ninad

❖ Life Sciences

214 Acharya Celin
215 Apte Shree Kumar
216 Badigannavar Anand M.
217 Ballal Anand D.
218 Bhilwade Hari Narayan
219 Chawla S. P.
220 Chittela Rajani Kant
221 Das Birajalaxmi
222 D'souza Stanislaus Francis
223 Fulzele Devanand Pralhadrao
224 Ganapathi T R
225 Ghosh Anu
226 Gopalakrishnan Roja
227 Jambulkar Sanjay J
228 Jamdar S. N.
229 Jha S K
230 Kulkarni Savita
231 Kulkarni Vishvas M
232 M G R Rajan
233 Makde Ravindra D.
234 Manjaya Joy G.
235 Maurya Dharmendra Kumar
236 Melo J S
237 Misra Hari S
238 Mukherjee Archana
239 Mukherjee Prasun Kumar
240 Mukhopadhyaya Rita
241 Nancharaiah Y. V.
242 Pandey B. N.
243 Patro Birija Sankar
244 R Shashidhar
245 Rajaram Hema
246 Rao T S
247 Rao T V C
248 Rath Devashish
249 Reddy kandali S.
250 Saini Ajay
251 Sainis Krishna Balaji
252 Santosh Kumar S.
253 Satyendra Gautam
254 Shankar Bhavani S.
255 Souframanien J.

256 Subramanian Mahesh
257 Suprasanna P
258 Toleti Subba Rao
259 Uppal Sheetal
260 Variyar Prasad S
261 Venugopalan V P
262 Banerjee Manisha
263 Bhat Nagesh
264 Chada Sonia
265 Das B K
266 Ghosh Sukhendu Bikas
267 Goswami Manish
268 Kota Swathi
269 Kumar Amit
270 Mehetre S T
271 Mishra Himanshi N
272 Saha Joshi Archana
273 Sharma Deepak

❖ Physical Sciences

274 Ahmed Zafar
275 Aswal Dinesh Kumar
276 Aswal V K
277 B.N. Raja Sekhar
278 Bakshi Ashok Kumar
279 Bandyopadhyay Tapas
280 Basu Saibal
281 Bera Santanu
282 Bhattacharya Debarati
283 Bhattacharyya Dibyendu
284 Bhattacharyya Soumen
285 Biswas Debabrata
286 Biswas Dhruba Jyoti
287 Biswas Dipak Chandra
288 Chandratre Vinay Bhaskar
289 Chaplot Samrath Lal
290 Chauhan Anil Kumar
291 Choudhury Narayani
292 Das Amitabh
293 Das Swapan
294 Debnath A K
295 Dev Vas
296 Dighe Priyamvada M
297 Dutta Debabrata
298 Dutta Dipanwita
299 Gadkari Sanjay C
300 Gaitonde D M
301 Ganesan Srinivasan
302 Garg Alka B
303 Ghorui Srikumar
304 Goswami Binoy Krishna
305 Gupta Anurag
306 Gupta N K
307 Jain Sudhir Ranjan
308 John Bency V
309 Kailas Swaminathan
310 Kannan Umasankari
311 Karmakar Debjani
312 Kaushik Trilok Chand
313 Koul Dileep Kumar
314 Kulkarni Mukund Shrinivas
315 Kumar Aniruddha
316 Kumar Mukesh
317 Kumar Vinay
318 Mahata Kripamay
319 Mazumder Subhashish
320 Mishra D. R.
321 Mishra Rosaline
322 Mitra Abhas Kumar
323 Mitra Subhankur
324 Mittal Ranjan
326 Mukherjee Goutam Dev
327 Mukhopadhyay Ramaprasad
328 Murli Chitra
329 Nakhate S G
330 Nayak Basanta Kumar
331 Nilaya J. Padma
332 Pant Lalit Mohan
333 Pradhan Swarupananda
334 Rajarajan A. K.
335 Ramaniah Lavanya
336 Rannot R C
337 Rao Divakar K.
338 Rao Mala N
339 Rao Pushpa M
340 Rao Rekha
341 Ravikumar G.
342 Ray Aditi
343 Renju George Thomas
344 Roy Bidyut Jyoti

345 Sahoo N K
346 Sahu Sanjay Kumar
347 Sakuntala T
348 Salunkhe Hemanth Govind
349 Sangeeta
350 Santra Satyaranjan
351 Sapra B K
352 Sastry U P
353 Saxena Alok
354 Selvam T. Palani
355 Sen Debasis
356 Shastri Aparna
357 Shrivastava Aradhana
358 Shukla Prashant
359 Singh Ajay
360 Singh Pitamber
361 Singh Surendra
362 Sucharita Sinha
363 Suryanarayana M. V.
364 Thakur Sanjay V.
365 Tickoo A K
366 Tripathi S. P
367 Udupa Dinesh Venkatesh
368 Wagh Pratap Baburao
369 Warrier Manoj Kumar
370 Yeram Shashwati Sen
371 Yusuf S M
372 Sinha Amar
373 Dasgupta Kamlesh
374 Chakraborty Keka R
375 Garg Nandini
376 Jayasekharn T
377 Kaur Manmeet
378 Kumar Munish
379 Saxena Vibha

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381 Batra Punita
382 Chakraborty Kalyan
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384 Dey Rukmini
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387 Raghavendra Nyshadham
388 Ramakrishnan B.
389 Ramana D. Surya
390 Ratnakumar P.K.
391 Shah Hemangi Madhusudan
392 Thangadurai Ravindranathan

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393 Basu Anirban
394 Bhattacharjee Jayanta Kumar
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396 Choudhury Tirthankar Roy
397 Das Tapas Kumar
398 Datta Aseshkrishna
399 De Aditi Sen
400 Gandhi Raj
401 Gopakumar Rajesh
402 Jatkar Dileep Prabhakar
403 Maharana Anshuman
404 Majumdar Pinaki
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461 Sudha C

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499 Venkatesan R.

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681	Mohapatra Ashok Kumar
682	Moulik Tania

683	Mykherjee Anamitra
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688	Srivastava Yogesh Kumar
689	Sumedha
690	Swain Sanjay Kumar
691	V. Ravi Chandra

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693	Nanda Dipankar

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695	Shukla Rahul

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717	Kumar Vinit
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720	Misra Pankaj
721	Modi Mohammed Hussein
722	Moorti Anand
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724	Mukhopadhyay P. K.
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739	Sinha A.K.
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743	Verma Sunil

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746	Hazra Montu K.
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749	Senapati Dulal

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752	Banerjee Subrata
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760	Raghuraman D. H
761	Saha Partha
762	Sarkar Munna (Ms.)
763	Sen Udayaditya
764	Sengupta Kaushik

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766	Avaroth Harindranath
767	Bandyopadhyay Bilwadal
768	Bandyopadhyay Debades
769	Banerjee Sangam
770	Basu Abhik
771	Basu Chinmay
772	Bhattacharjee Pijushpani
773	Bhattacharya Satyaki
774	Bhattacharyya Gautam
775	Bhattacharyya S. R.
776	Bhunia Satyaban
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779	Chakraborty Supratic
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783	Das Indranil
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811	Mohanty Pradeep Kr.
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825 Roy Pradip Kr.
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827 Roy Subinit
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829 Sarkar Maitreyee Saha (Ms.)
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831 Sarkar Subir
832 Satpati Biswarup
833 Sharan Manoj K.
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1000	Dutt Shilpee (Ms.)
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1005	Mahimkar Manoj Balkrishna
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1017	Nabhiraj P. Y.
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1038	Ghosh Tilak Kumar
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1050	Srivastava Dinesh Kumar
1051	Zubayer Ahammed

Section-II

Scientific and Technical Achievements During Present Period Through Completed Ph. D. Work

Highlights of Research Conducted by HBNI Doctoral Students (2016-17)

1. Physical Sciences

During this period, HBNI awarded Ph.D. degree to 75 students who carried out research in the area of Physical Sciences at different CI/OCC of HBNI. Highlights of these doctoral research works specific to different CI/OCC are as follows.

1.1 Bhabha Atomic Research Centre (BARC), Mumbai

At present there are about 150 Ph. D. students pursuing their doctoral programme in Physical Sciences in BARC. During the period 16 students have been awarded Ph.D. degree covering a wide range of topics. Brief highlight are given in the following paragraphs.

There are several theses that deal with major instrumentation programme in DAE involving utilization of synchrotron sources viz. Indus 1 and Indus 2. The theses of Ashwani Kumar deals with the development of Protein crystallography beam line in Indus 2. Himal Bhatt has worked on the development of the infrared beam line in Indus 1 and Ashish Agarwal has worked on development of x-ray and neutron imaging techniques using Indus 2 and neutron sources. Fig 1.1.1(a) shows the schematic of the protein crystallography beam line and Fig. 1.1.1(b) shows the cartoon of a protein monomer, whose structure has been solved using this beam line data.

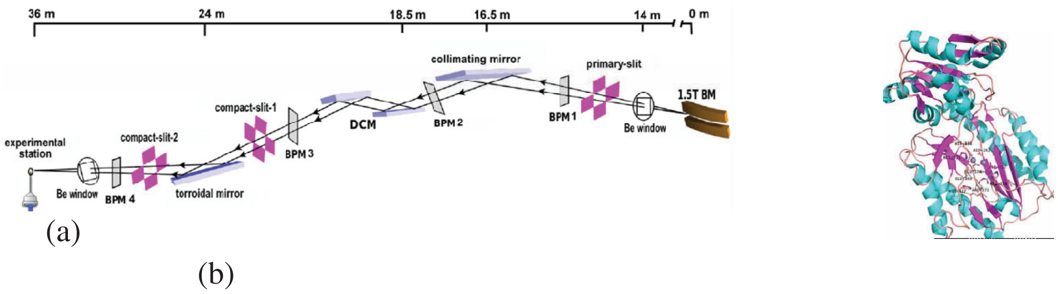


Fig. 1.1.1. (a) Schematic of Protein Crstallography beam line and (b) Cartoon of a PepQxc monomer obtained from the data obtained on the beam line

The infrared beam line sample station in Indus 1 is shown in Fig. 1.1.2 (a) and the high pressure data collected from beam line sample station for oxalic acid is shown in Fig.2 (b)

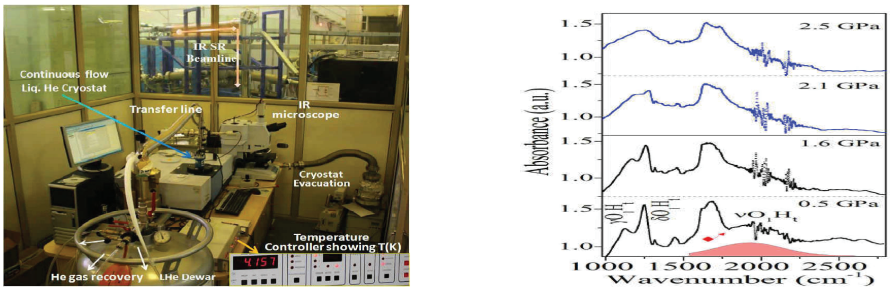


Fig. 1.1.2 (a) Infra-red bam line sample station and (b) High pressure data from oxalic acid in Indus 1

X-ray and neutron imaging are two important complementary techniques for various industrial samples. Ashish Agarwal has developed various formalisms and also worked on the imaging beam line to obtain x-ray image (Indus 2) and neutron image (CIRUS). Fig. 1.1.3 (a) Shows the experimental station of the x-ray imaging facility at Indus 2 and Fig. 1.1.3(b) shows 3 dimensional re-constructed image of a bone taken on the beam line

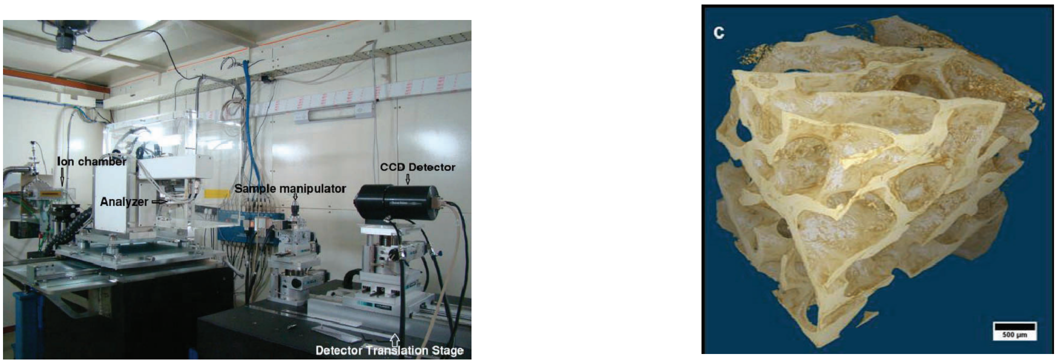


Fig. 1.1.3 (a) X-ray imaging beam line (INDUS2) (b) Reconstructed image of a bone done on the beam line data

There have been two major gamma ray telescope projects in DAE, TACTIC and MACE. One is located at Mount Abu in Rajasthan and the other at Hanle, Ladakh. The thesis of K. K. Singh has dealt with the observation of very high energy gamma rays using TACTIC. Mradul Sharma has worked on data analysis for the MACE telescope at Hanle in Ladakh India. This telescope is now under installation and Mradul has simulated data to test the feasibility of experiments at this telescope. Fig. 1.1.4 shows the TACTIC telescope with its instrument panel at Mt. Abu.

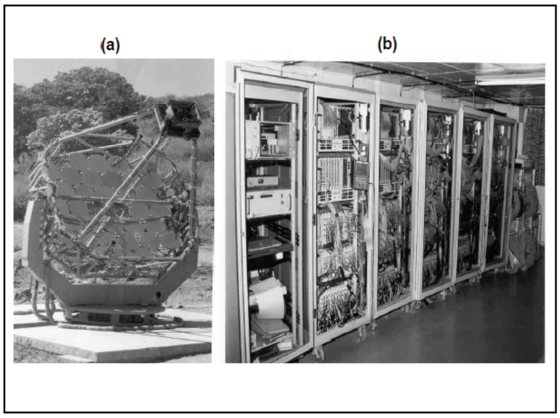


Fig. 1.1.4 TACTIC Telescope at Mount Abu, Rajasthan with its instrument panel

There have been several theses on various issues related to design of the Indian Neutrino Observatory (INO). This is another major experimental project on fundamental physics being pursued by the department. A large number of INO students, scattered in various CI's of HBNI are pursuing their Ph. D. under this project are under BARC. There have been five theses during last year that dealt with Ph. D. in various experimental and simulation studies being carried out for the INO project. These are (a) Ms K K Meghna on "Performance of RPC detectors and study of muons with the Iron Calorimeter detector at INO" (b) Shri Shiba Prasad Behera on "Electromagnetic Simulation of NON-ICAL Magnet and its Sensitivity to Sterile Neutrino Mixing", (c) Shri Varchaswi KS Kashyap on "Studies on Resistive Plate Chambers (RPC) for INO and scintillators for reactor antineutrino detection", (d) Ms Ali Azmi on "A study of moonless events and an attempt to improve the hierarchy sensitivity through neural networks at ICAL@INO", (e) Ms Nitali Das on "Feasibility studies for the detection of exotic particles using ICAL at INO".

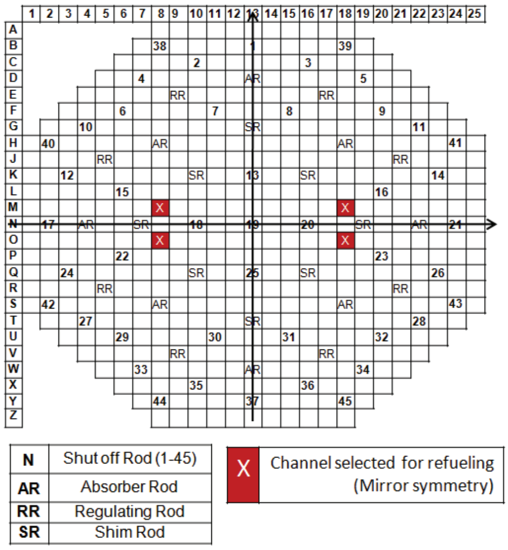


Fig 1.1.5: Schematic of AHWR Core

Neutronics calculations and simulations are important for various types of neutron sources and for fissile or fertile materials. Amit Thakur's thesis on "Development of Optimization Techniques for Fuel Management in Heavy Water Moderated Reactors" has been an attempt to improve fuel economy in a heavy water reactor. Sadhana Mukherjee's thesis on "Neutron Induced Cross Section and Fission Yield Measurements for Thorium and Uranium" has reported studies on these two extremely important materials for our programme. Rajeev Kumar has attempted a new technique of reactivity calculation in his thesis entitled "Measurement of reactivity in sub-critical reactors using neutron noise methods". Both Amit Thakur and Rajeev kumar have dealt in details with the neutronic in Advanced Heavy Water Reactor or AHWR core. The schematic of the core is shown in Fig. 1.1.5.

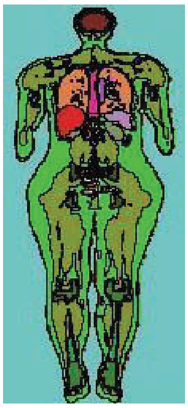


Fig. 1.1.6: ICRP reference adult male voxel phantom

Radioactivity and its use in diagnostics as well as in therapy are important research activities under HBNI. These activities have large societal impact. Minal Nadar has btained her Ph. D. on in-vivo radioactivity measurements. Sudhir Kumar carried out Monte Carlo based dosimetry calculations in his doctoral work. Fig. 1.1.6 shows an ICRP standard male phantom used by the above workers for their dose estimation and simulations.

Development of mass spectrometers has been an important activity in BARC. R.K. Bhatia has described development of Development of Magnetic Sector Mass Spectrometers for Isotopic Ratio Analysis in his thesis. Fig. 6 shows a quadrupole ion trap developed by him during his doctoral work.

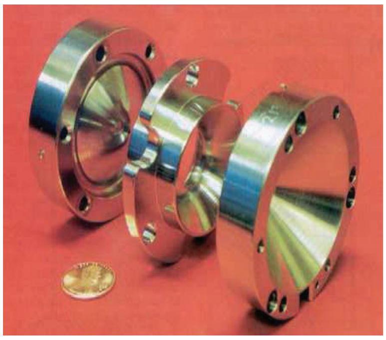


Fig.1.1.7. A quadrupole ion trap for mass-spectrometer

A large number of neutron spectrometers have been are available at Dhruva reactor for neutron beam research. Sumit Mehan has studied Nanoparticle Effect on Structural Evolution of Protein-Surfactant Solutions using Small Angle Neutron Scattering (SANS) at Dhruva. Fig. 1.1.8 shows a schmetaic of a mixture of protein nanoparticles and surfactants and the type of physical structure they form.

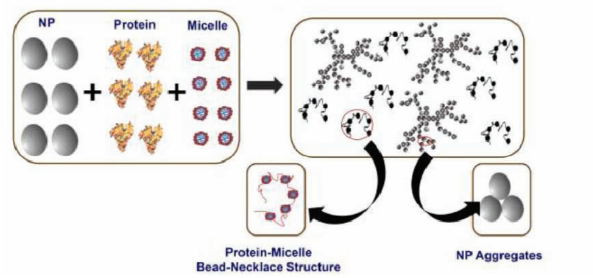


Fig. 1.1.8: Schematic of the structures formed in protein-nanoparticle-surfactant three component systems

The thesis of B.M. Kukreti on "Radiometric studies to understand disequilibrium of uranium across a few exploratory blocks of Mahadek basin, Meghalaya and its implication on uranium exploration" is important for Uranium exploration in the North-Eastern part of India. Mahadek basin has geological potential of having medium and small pockets of U_3O_8 disposed at shallow depths. The thesis presents an important work on Uranium prospecting in the country. Fig. 1.1.9 shows a geological map of the Mahadek basin in Meghalaya Plateau. The thesis primarily deals with this region.

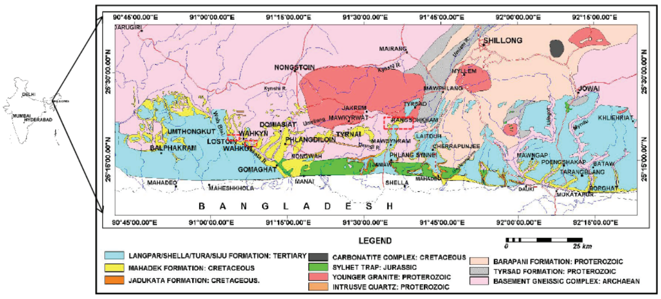


Fig. 1.1.9: Mahadek basin with geological map

The thesis of A. Sai Venkata Ramana has worked out a formalism of using Global Renormalization Group Theory (GRST) to obtain Equation of State (EOS) for liquid-vapour phase transition. His work has important implications for high-energy density physics. Apart from hydrodynamic approach this technique is quicker for obtaining EOS.

1.2 Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam

During the period, 9 students were awarded Ph.D. degree in Physical Sciences. Highlights from some the theses are presented as follows.

Diamond Like Carbon (DLC) films, owing to their unique properties includes high hardness, ultra-low friction coefficient and extremely high wear resistance have become an obvious choice for electronic, optical and wear protection applications in nano to micro and macro-scale. Ultra smooth DLC films were grown on single crystal Si (100) substrates using plasma enhanced CVD technique as a function of substrate bias and nitrogen doping. The bonding, chemical structure and hydrogen content of these films were evaluated as function of the ion energy and nitrogen doping concentration. The variation in local elastic modulus of DLC films as a function of ion energy and nitrogen concentration was demonstrated by the acoustic force atomic microscopy. This provided the microscopic evidence for the graphitic phenomenon explained by the established sub-implantation growth model for DLC films. The measured elastic modulus of the films was well corroborated with the structural properties. Further the friction coefficient and wear rate of these films deposited as function of substrate bias and nitrogen concentration were obtained and correlated with bonding, film density and hydrogen content. Moreover, a detailed surface analysis using X-ray Photoelectron spectroscopy signified the role of adsorbed oxygen layer in controlling friction and wear properties. Additionally the sliding induced structural transformations also demonstrated using Raman spectra mapping of the wear tracks. This work provided an insight on various mechanisms governing the friction and wear depends on the test environment. The role of surface passivation and sliding induced graphitization in achieving super low friction and high wear resistance was substantiated. In this work we also achieved DLC surfaces with tunable wetting characteristics. Finally, the work summarized the influence of surface chemistry on tribological properties of DLC films.

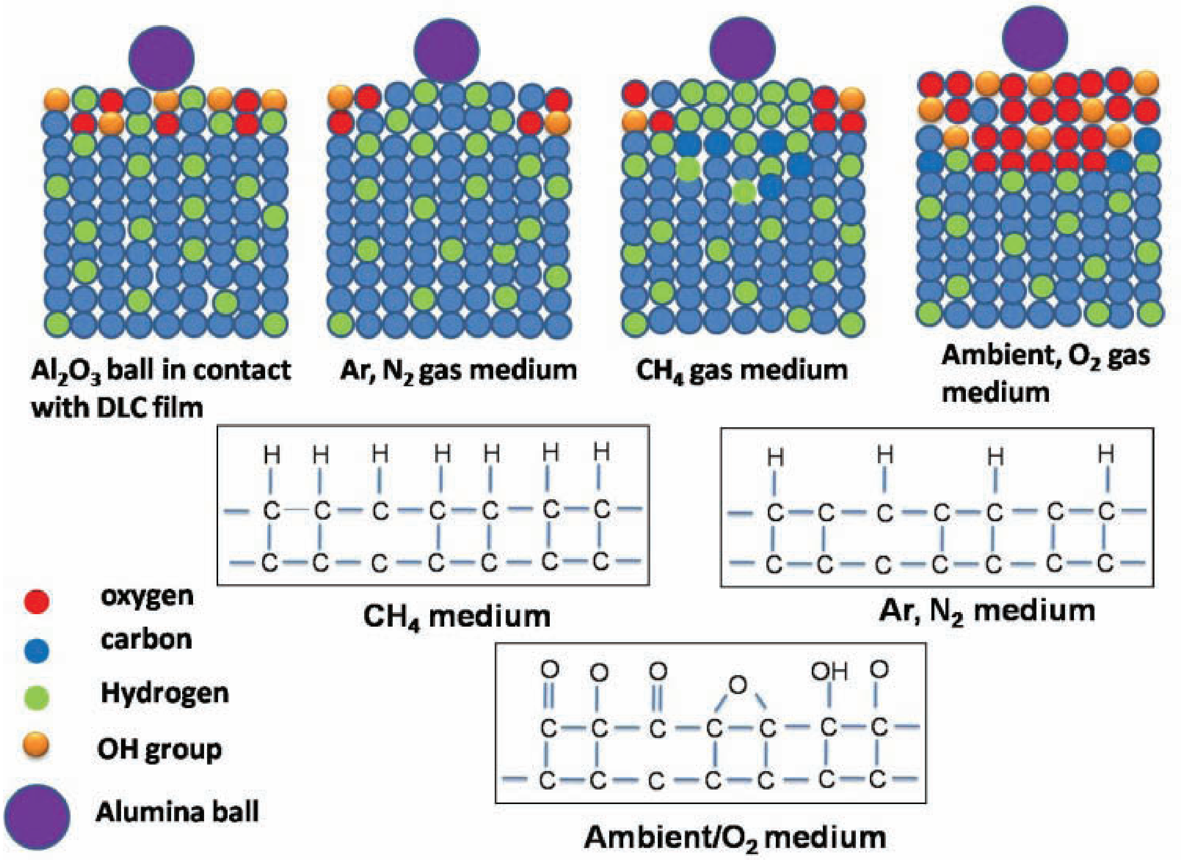


Fig. 1.2.1 Schematic of tribo-chemical reactions at DLC surfaces tested in various gas medium

Ti alloys gain attention in the last 4-5 decades for their applications in areas such as the biomedical field to aerospace engineering due to its unique combination of properties like high strength to weight ratio, biocompatibility, and corrosion resistance. Identification of non equilibrium transformation products of Ti-Mo alloys using conventional and synchrotron X-ray Diffraction (XRD) and understanding the microstructure variations of the same, using microscopy techniques like SEM and TEM. Rietveld refinement XRD pattern to arrive, crystal structural details of non equilibrium transformation products. This includes lattice parameter, atom positions, coordination number, bond length, and the bonding characteristics. Investigation of phase transformation mechanisms/products in Ti-1Mo and Ti-7Mo alloys at various cooling conditions. The alteration of transformation mechanism from non-diffusional to diffusional has been studied with microstructural analysis and crystal structure details. The possibility of variant selection mechanism is analyzed using orientation imaging microscopy (EBSD/SEM and PED/TEM). The signatures of athermal and isothermal ω phase formations, the lattice collapse mechanism during its formation and its distribution in the β matrix have been studied in detail in Ti-15Mo alloys with HRTEM and inverse FFT techniques. Rietveld refinement of the XRD pattern confirms the lattice parameter and relative volume fraction of hcp α, bcc β and hexagonal ω phase in the aged Ti-15Mo alloys. The retrieval of structure factor details from the XRD pattern confirms the electron charge density distribution of the ω phase in space and predicted “graphite like bonding”.

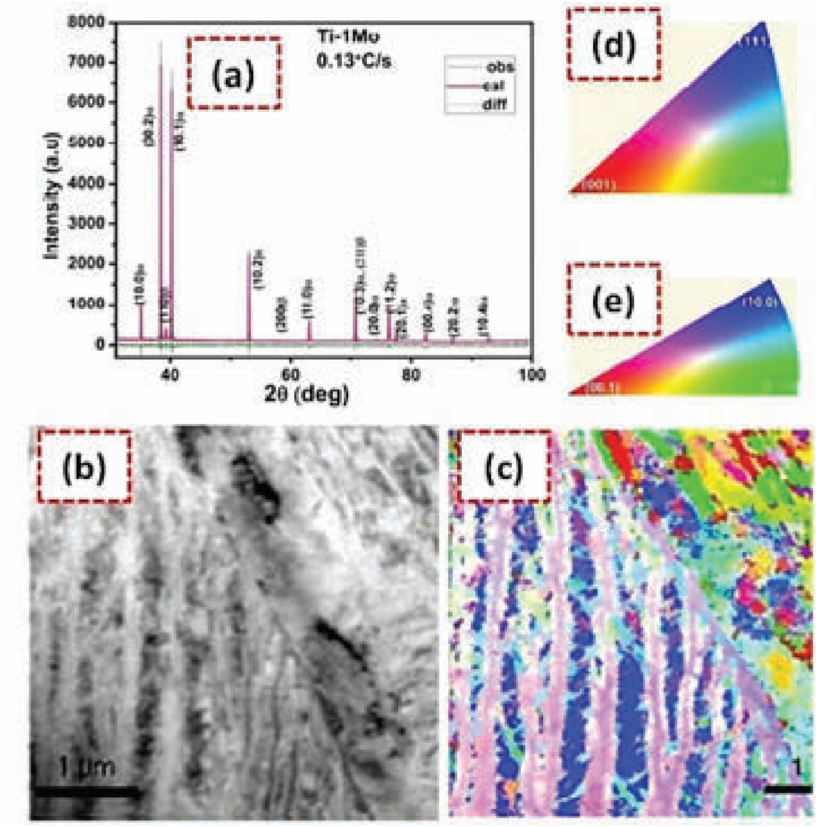


Fig. 1.2.2 (a) Rietveld refined XRD pattern showing the formation of α and β phase, (b) BF image showing Widmanstatten structure (c) Orientation map of same region and (d) and (e) represent IPF color codes of $\beta$and α phases in Ti-1Mo at a cooling rate of 0.13 ^{o}C/s.

Anharmonic effect is usually very strong in two dimensional (2D) crystals and it becomes more pronounced at high temperatures. After the discovery of graphene, researchers studied the structural and thermodynamic properties of different 2D materials in detail using harmonic, quasi-harmonic (QH) and anharmonic lattice dynamics (LD) methods. All the above methods fail to capture the true anharmonic nature of 2D materials. To compute the structural, thermal and vibrational properties of 2D materials with full anharmonicity of effective interaction between atoms, we developed a spectral energy density (SED) method and implemented in classical molecular dynamics (MD) simulation package LAMMPS. Using this method, we computed the temperature dependent structural stability, frequency shift, linewidth and coupling of normal modes of vibrations of graphene, 2D h-BN and monolayer (ML)-MoS2. The results obtained show significant difference from quasi-harmonic studies due to the inclusion of higher order phonon-phonon coupling processes, which were absent in quasi-harmonic approximation. The structural stability analysis envisages that the inclusion of higher order phonon-phonon coupling is a must to stabilize the graphene and 2D h-BN sheet at finite temperatures. Unlike graphene and 2D h-BN, in ML-MoS2, its finite thickness effect counteracts against the membrane effects and makes the crystal stable and prevents the crumpling transition. We delineated the contributions of thermal expansion and anharmonic coupling of phonon modes to the frequency shift and linewidth, and found that theanharmonic coupling of phonon modes is the dominant source of observed frequencyshift and broadening of peaks.

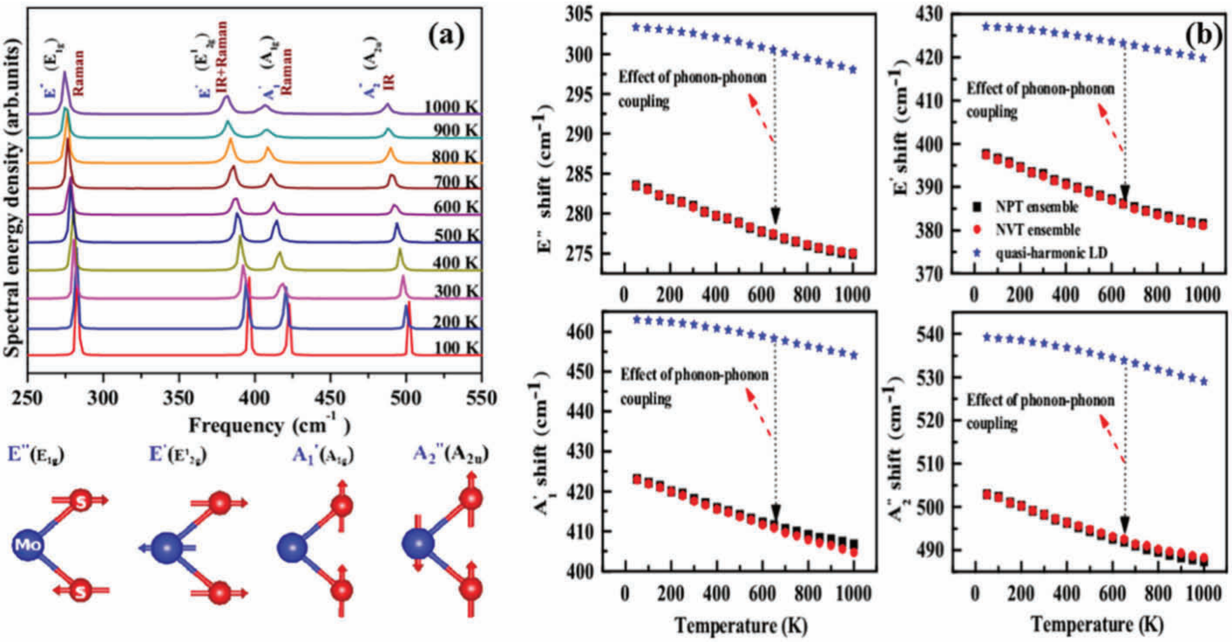
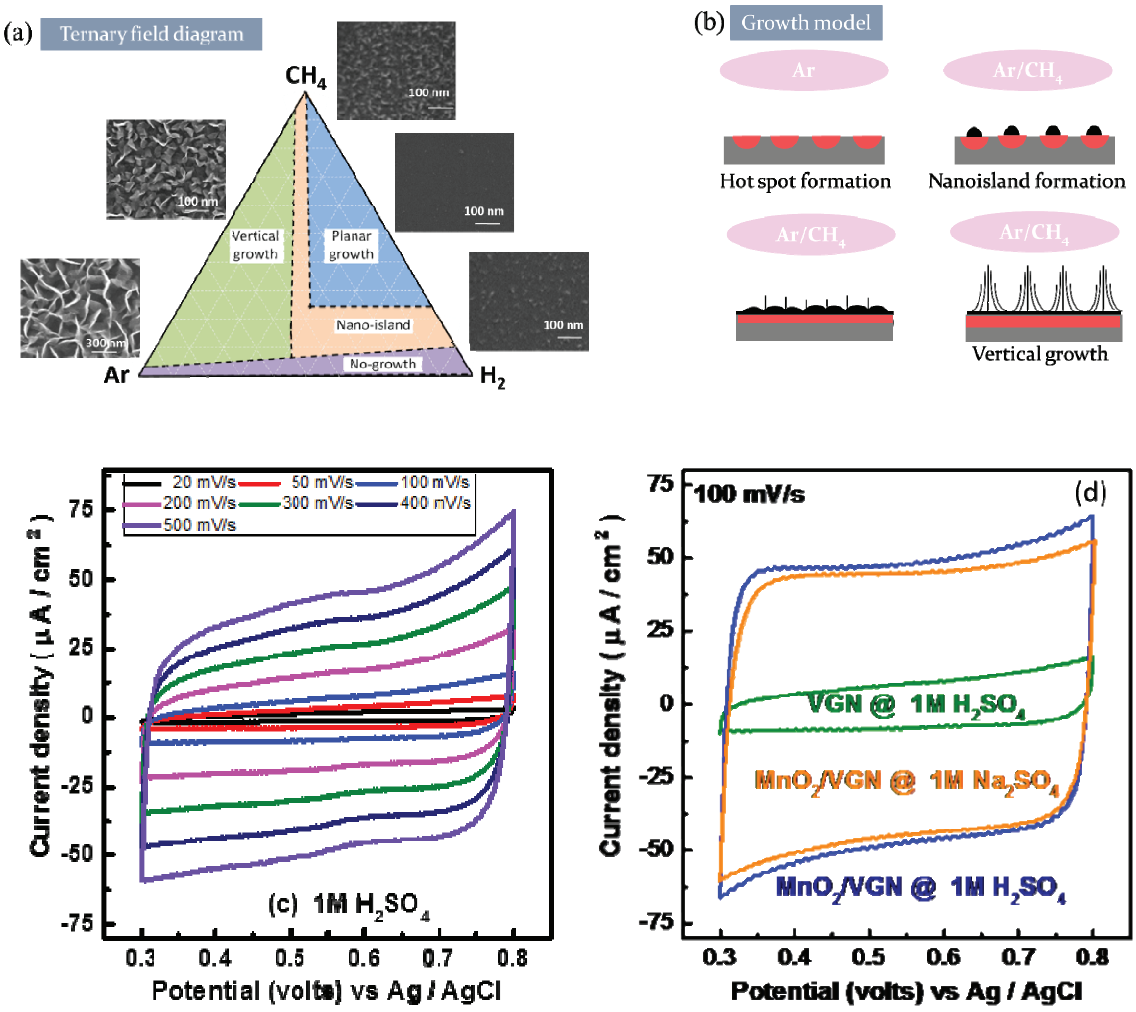


*Fig. 1.2.3 (a) (Top) the Γ-point optic phonon modes as a function of temperature. The modes are labeled according to factor group analysis (the notations inside the bracket correspond to bulk representation). Infrared (IR) and Raman active modes are indicated. (Bottom) Eigenvectors of the corresponding modes.**(b)**The temperature dependent peak shifts of Γ point optic modes in ML-MoS*$_2$*. The quasi-harmonic lattice dynamics (blue-stars) calculations include only the effect of thermal expansions. The NVT ensemble mode frequency shift (red spheres) is purely due to the anharmonic coupling of phonon modes. The NPT ensemble mode frequency shift(black squares) contains the combined effect of thermal expansion and anharmonic coupling of phonon modes.*

Due to unique geometry, high surface area, good electrical conductivity and three-dimensional network, vertical graphene nanosheets (VGNs) received strong momentum towards its wide range of applications. To utilize them in potential application, a clear understanding of growth mechanism and optimization of growth parameters to achieve desired morphology is highly essential. With this motivation, the present work addressed towards synthesis and studies of VGNs and their application towards supercapacitor (SC) electrode. A systematic study on synthesis of VGNs using plasma enhanced chemical vapor deposition is carried out. The effect of growth time, feedstock gas composition, growth temperature, microwave power, distance from plasma to substrate and role of substrates on growth and structural properties of VGN are addressed. The experimental observations reveal the tunable morphology from vertical to planar structure by changing growth parameters. Based on the observed results a ternary field diagram of nanographitic structure is established. A phenomenological four stage growth model is proposed and discussed, to substantiate the defect-induced nucleation and growth mechanism of VGNs by invoking substrate-plasma interaction during growth. Finally, supercapacitative behaviour of the VGNs under aqueous electrolytes (Na2SO4, KOH, and H2SO4), were conducted using three electrode system. An electrical equivalent circuit modelling is performed based on electrochemical impedance spectroscopy to elucidate electrolyte-electrode interaction. H2SO4 is found to be a choice of electrolyte in terms of specific capacitance, cycle life, efficiency and time constant. Integration of VGNs with MnO2 is a promising to further enhance the capacitance of VGN sowing to its fast redox kinetics, less toxicity and less expensive. In addition to enhancement in capacitance of composite by five times, VGNs is found to serve as excellent mechanical backbone for the effective utilization of MnO2 without any structural degradation. Obtained results demonstrate that the VGNs and its composites can be a potential candidate for SC applications.



Stimuli responsive microgel particles are micron/sub-micron sized hydrogel particles which respond to external stimuli like temperature, pH, ionic strength, etc., by undergoing swelling or de-swelling transitions. Poly (N-isopropyl acrylamide) (PNIPAM) and Poly (N-isopropyl acrylamide –co- acrylic acid) (PNIPAM-co-Aac) microgels are few well-studied microgel systems. These particles are soft, compressible and core-shell structure with densely cross-linked core and loosely cross-linked shell. These microgel particles exhibit large change in their size at a particle value of external stimuli known as volume phase transition (VPT). Conventionally, dynamic light scattering (DLS) technique was used to identify the VPT of microgel particles which required ~ 107 particles / cm3. Due to inherent nature of microgels (varying cross-linker density across the particle) and size polydispersity of the sample, VPT is always shown to be a continuous transition (second order transition) instead of sharp transition (first order transition) as predicted by Flory-Huggins theory. Since VPT is the property of polymer itself,

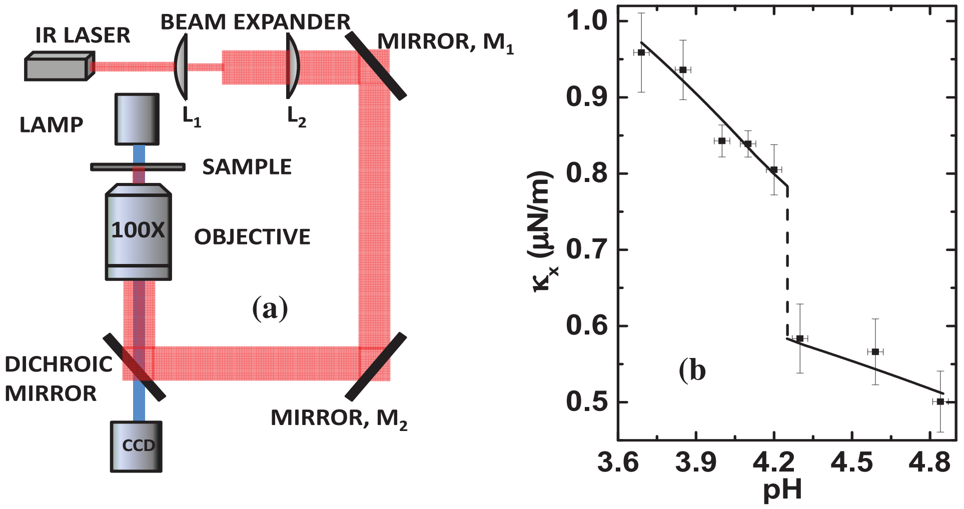


Fig. 1.2.4 (a) Schematic of optical lay out of the optical tweezers set-up. (b)Trap stiffness, κ_x *measured as a function of pH on a single microgel particle using optical tweezers. Continuous line denotes the numerically computed,* κ_x *using OTCT. Dashed line represents sudden change in* κ_x *occurring at VPT.*

measurement of VPT on a single particle with give us more insight about the transition. Towards that, we have indigenously designed and developed optical tweezers set-up coupled with 1064 nm laser for trapping (Fig. 1.2.4 a). For the first time, we have shown that a single low refractive index contrast microgel can be trapped. We have used optical tweezers to investigate the VPT of PNIPAM-co-Aac microgel particle as a function of pH. Trap stiffness as a function of pH was measured and it showed a sudden jump at pH 4.20 which is identified as VPT (Fig. 1.2.4 b). We numerically calculated the trap stiffness as a function of pH which qualitatively agrees with the experimental results. Sudden jump in the trap stiffness is understood to arise due to sudden decrease in particle size and concomitant increase in the refractive index of the microgel particle. Hence, we have shown that optical tweezers can be used to identify the VPT on a single microgel particle and serve as an alternative technique to DLS.

The future of nuclear power depends on the safe operation of nuclear power plants. New reactor design concepts are being developed to improve the safety aspects of nuclear power plants. The new reactor design concepts work on the principle of inherent safety features and passive safety features. These safety features challenge the traditional decoupled safety analysis approaches of deterministic and probabilistic safety analysis. The IDPSA methodologies integrate both deterministic and probabilistic safety analysis. IDPSA methods in general are referred as dynamic reliability. Dynamic reliability involves modelling the time dependent behaviour of both physical process and safety system hardware. A suitable Monte Carlo simulation scheme for the time dependent behaviour of system hardware is identified in this thesis. This is achieved by applying different MC simulation methods on a typical reactor safety system. The identified Monte Carlo simulation scheme is combined with a physical decay heat evolution process and the probabilities of crossing different critical temperature limits are estimated.

The conditions under which classical PSA approaches and dynamic reliability approaches lead to same / different results is one of the open issues. An attempt to understand this condition is made in this thesis. The probability of crossing the different temperature limits is estimated for different process uncertainties. The results from classical and dynamic approaches are significantly different when the process uncertainty contribution to total failure probability is not dominant and results converge when the process uncertainty contribution to total failure probability is dominant. This is illustrated in fig.1.2.5.

In Sodium Fast Reactors, the sodium metal aerosol characteristics present in the cover gas region is important to understand the heat and mass transfer to the roof top and side wall, visibility of cover gas region, design of purification system efficiency, aerosol deposition to roof top and its penetration, convection velocity in cover gas region and fission product scavenging by these aerosols. Development of theoretical models and their verification on specific experimental results remain necessary to determine/estimate sodium aerosol mass concentration and sodium aerosol size distribution in cover gas region. In this regard, experimental and theoretical studies are carried out in SILVERINA loop at FRTG and characteristics of sodium metal aerosol in cover gas region determined, for various sodium pool temperatures, different heights of cover gas region, different geometry and under gamma radiation condition. The sodium metal aerosol size (MMD) and mass concentration in cover gas region is ranges

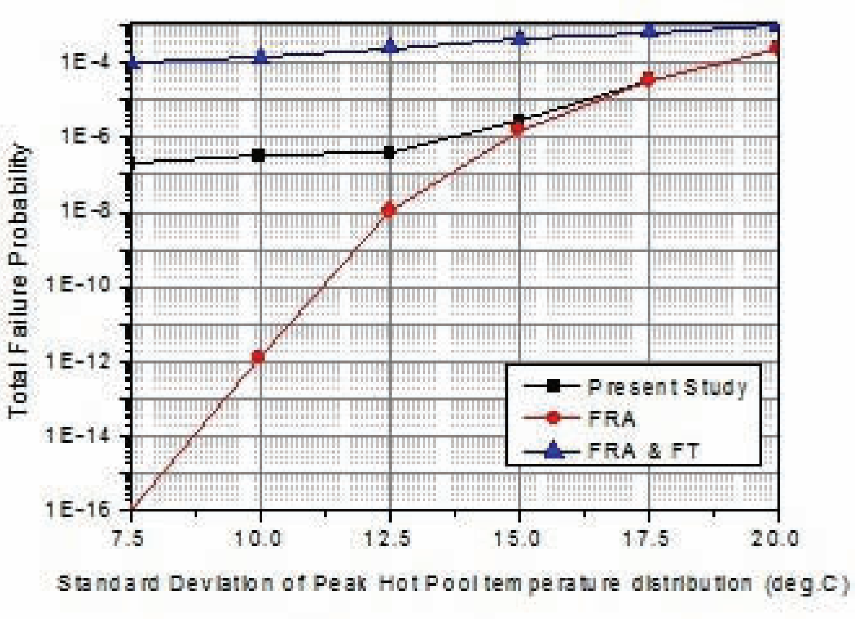


Fig.1.2.5. Convergence of classical PSA (curve FRA & FT in fig) results and dynamic PSA results (curve present study in fig) as a function of process uncertainty contribution (curve FRA in fig) to total failure probability.

from 1.5 µm to 16 µm and 0.026 g/m^3 to 35.55 g/m^3 respectively for sodium pool temperature 250^{o}C - 550^{o}C. The MMD and mass concentration increases with increase of sodium pool temperature for a given geometry. The MMD of sodium metal aerosol size is larger and mass concentration is more near the sodium pool compared to that of the middle level of cover gas region and near the roof for a given geometry. The MMD of sodium metal aerosol increases and mass concentration of sodium aerosol decreases with the increase of aspect ratio (L/D, L – height and D – diameter) of cover gas region. The MMD of sodium metal aerosol is found to be higher and mass concentration is found to be less in the presence of gamma field when compared to that of without gamma field condition. The study is found to be useful for prediction of sodium metal aerosol characteristics in cover gas region for aspect ratio 0.55 ≤ L/D ≤ 4.52 and for the sodium pool temperature 250^{o}C ≤ Tp ≤ 550 ^{o}C.

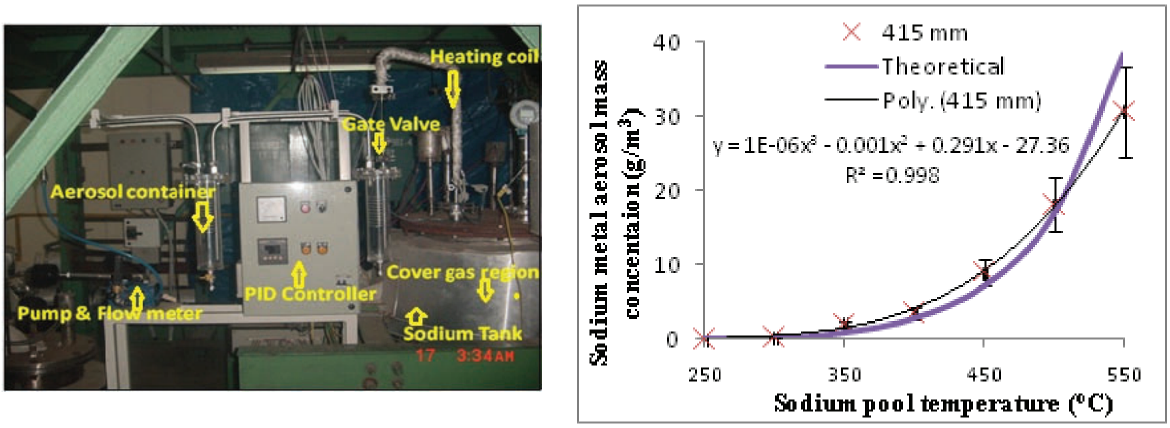


Fig 1.2.6. Photograph of sodium metal aerosol sampling system and sodium metal aerosol mass concentration (theoretical and experimental) for various sodium pool temperature.

Motivation behind the thesis is to explore the deposition feasibility of piezoelectric a-axis oriented AlN thin films by IBSD under reactive assistance of N^+/N_2^+ ions and subsequent measurement of their piezoelectric response by different techniques. For this,(i) Growth kinetics of AlN thin films has been investigated using dynamic scaling theory (DST) to delineate the role of N^+/N_2^+ ions on growth characteristics. (ii) Deposition parameters were optimized for the growth of a-axis textured wurtzite hexagonal AlN thin film on Si(100) substrate. (iii)Theirmorphological, structural and compositional analyses have been carried out using an array of analytical techniques like atomic force microscopy (AFM), scanning electron microscopy (SEM), X-ray diffraction (XRD), high resolution transmission electron microscopy (HR-TEM),X-ray photoelectron spectroscopy (XPS) and UV-VIS

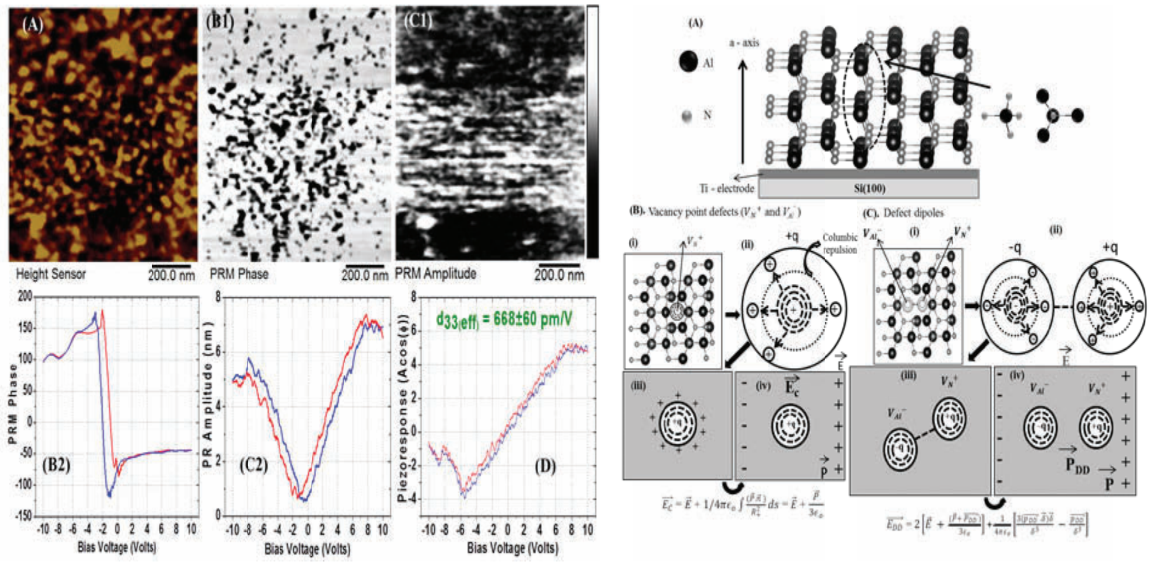
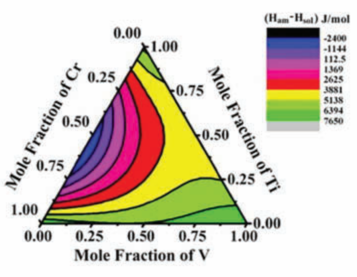


Fig. 1.2.7. Left: Piezo force microscopy (PFM) results of IBSD grown a-axis oriented AlN thin films, (A) Height scan, (B1), piezo response phase image, (C1), piezoresponse amplitude image, (B2) electrical hysteresis, (C2) mechanical hysteresis (butterfly loop), (D) piezoresponse loop exhibiting high longitudinal piezoelectric coefficient $d_{33(eff)}$.

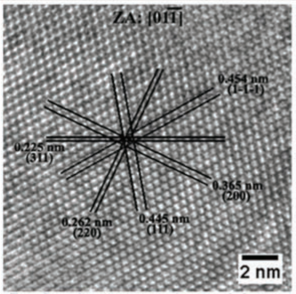
Right: Model for charged vacancy induced enhancement in lattice polarization, (A) a-axis oriented AlN/Ti/Si(100) hetrostructure, (B) and as spherical cavities in a dielectric, (C) Formation of defect dipoles by the presence of two spherical cavities of opposite surface charge at the nearest possible distance.

spectrophotometry. Presence of defects in film microstructure was investigated with positron annihilation and photoluminescence (PL) spectroscopies. (iv) Piezo response of IBSD grown a-axis oriented AlN thin films was explored using three different techniques. These are, (i) Piezo Force Microscopy (PFM) - an atomic force microscope (AFM) based technique. Piezo response loops were obtained to find out effective values of longitudinal piezoelectric coefficient *($d_{33(eff)}$)*, (ii) Capacitance-Voltage (C-V) measurements on Ti/AlN/Ti/Si(100) capacitive hetrostructures. (v) The measured values of piezoelectric coefficient $d_{33(eff)}$ for these samples are as high as 206 ± 20 pmV^{-1} and 668 ± 60 pmV^{-1} calculated by piezo response loop for AlN films of a thickness of 235nm and 294 nm respectively.(vi) A suitable model is proposed to explain these high $d_{33(eff)}$ values for IBSD grown, a-axis oriented AlN thin films, based on charged defects induced enhanced polarization in the dielectric continuum of AlN.

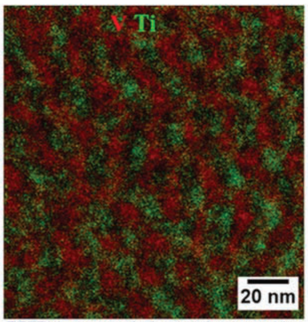
Figure below provides a pictorial representation of the thesis entitled "Phase Stability and Microstructural Evolution in V-Ti-Cr System Using Phase Contrast, HAADF Imaging and Electron Spectroscopy". Thermodynamic calculations based on Miedema approach were instrumental to study the phase stability of V-Ti-Cr alloy system. Phase contrast microscopy aided with multislice simulation was carried out to understand the V-atom occupancy in V-substituted $TiCr_2$ Laves phase. Composition modulation through Spinodal decomposition and the subsequent ω phase formation in equiatomic V-Ti and V-Ti-20Cr alloys as well as their structural imaging were important aspects of the thesis.



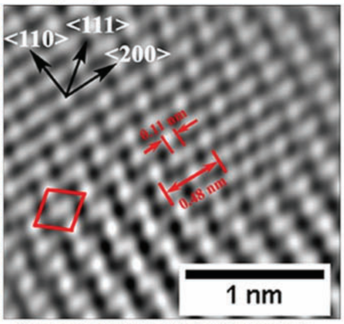
Enthalpy contour plot as calculated from Miedema model over the entire composition range of V-Ti-Cr



Zero-loss phase contrast micrograph from V-substituted $TiCr_2$ Laves phase alloy along [0 1 -1] zone axis



EFTEM micrograph showing the composition modulation from a Spinodally decomposed region in binary V-50Ti alloy



Phase contrast micrograph showing the atomic arrangement in a partially collapsed ω structure

1.3 Raja Ramanna Centre for Advanced Technology (RRCAT), Indore

During academic year 2016-17, four scholars have been awarded Ph. D. degree by HBNI in the discipline of Physical Sciences. Some of the salient points of these theses are given below:

A study on the effect of doping on the temperature dependent electron transport in intrinsically and / or extrinsically doped ZnO thin film grown by atomic layer deposition (ALD) has been carried out for a Ph. D. thesis work. It has been found that electron transport in these films is driven by the intricate interplay of screening and disorder. The temperature dependence of phase-coherence length, as extracted from the magnetoresistance measurements, indicated inelastic electron-electron scattering as the dominant dephasing mechanism in these dirty metallic systems.The temperature dependent photoluminescence and room temperature optical absorption spectra were found to be in good conformity with the combined effects of Burstein-Moss band filling and band gap narrowing above Mott critical density of ZnO.

A thesis devoted to the investigation of structure and spectroscopic properties of transition metal based magneto-electric multi-ferroic systems and their correlation with the magnetic as well as ferroelectric properties was awarded Ph. D. degree. This thesis reported synthesis of low structural symmetry systems Co3TeO6(CTO) and Mn doped CTO (CMTO) using an optimized solid state reaction route and their growth mechanism was studied. Further, cobalt is found to exist in mixed oxidation states of +2 and +3, which gives rise to the possibilities of both ferromagnetic (FM) and antiferromagnetic (AFM) interactions, in CTO. With the help of low magnetic field magnetization, it is established that CTO show short range FM interactions in addition to AFM interactions, the so called Griffiths Phase (GP). Experimental observations of spontaneous polarization as well as spontaneous magenetization and magneto-dielectric coupling (representing spin lattice coupling in this system) have been reported in CTO, for the first time.

Raman spectroscopy/mapping and atomic force microscopy mapping (AFM) have been employed to investigate properties of two nanocomposites (NCps): (i) Si-SiO2 (ceramic matrix) and ii) CdS-polyvinyl pyrrolidone (PVP: polymer matrix). In Si-SiO2 NCps grown by pulsed laser deposition, large variation (495 - 519 cm-1) in Si phonon frequencies was shown to arise from surface/interface of smaller Si nanocrystal and core of larger Si nanocrystals dispersed in SiO2 matrix. Raman spectroscopy/mapping study showed that the interface between Si nanocrystals and SiO2 plays an important role in Raman spectra. Further, it was found that the resonance Raman scattering is crucial for the observance of these surface/interface phonons. Further, in corroboration with AFM reveals stacking of different size Si nanocrystals in clusters of Si-SiO2. Similarly, in CdS-PVP NCps, it is found that the interaction between CdS nanocrystal surface and PVP monomers gives rise to collapse of polymer, which in turn leads to formation of nearly monodispersiveCdS nanocrystals embedded in PVP spheres. Thus, it is found that interaction between semiconductor nanocrystal and matrix plays an important and distinctive role in determining the morphology and properties of NCps.

Effects of disorder on electrical and optical properties of doped ZnO thin films grown by pulsed laser deposition (PLD) were investigated experimentally. It was found that Si can be used as an n-type dopant in ZnO for transparent conducting electrode (TCE) applications as Si lowered the resistivity of ZnO films to ~ 4.6×10-4 ohm-cm with about 80% transmission in the visible spectral region. Si doping related defects was found to cause semiconductor to metal transition, bandgap narrowing and PL broadening. It was found that temperature dependent resistivity behavior of the Si doped ZnO films could be explained by considering disorder induced quantum corrections to the Boltzmann's conductivity, which includes the effect of weak localization (WL) and electron-electron interactions (EEIs). In presence of disorder the electron mean free path becomes comparable to the electron Fermi wavelength and electron interference effect shows up as quantum corrections to conductivity in the low temperature transport properties. A metal to semiconductor transition occurred was observed in these degenerately Si doped ZnO thin films as the thickness of the films was reduced from 40 to 15 nm. Effects of disorder on optical and transport properties of 2D electron gas (2DEG) formed at the interface in MgZnO/ZnO interface was also studied. Due to the presence of disorders, electron interference effects resulted in logarithmic dependence of conductivity of 2DEG on temperature.

1.4 Variable Energy Cyclotron Centre (VECC), Kolkata

During the period, 7 students were awarded Ph.D. degree in Physical Sciences. Highlights from some the theses are presented as follows.

Nuclear Multifragmentation is an important area of research where an excited system is formed in collision between two nuclei and when its excitation energy is greater than a few MeV per nucleon, it breaks into many nuclear fragments of different masses. In order to study nuclear multifragmentation theoretically as well as to explain relevant experimental data we have developed statistical and dynamical models. Using these models we have studied (i) production of exotic nuclei which are normally not available in the laboratory (ii) nuclear liquid-gas phase transition and (iii) nuclear symmetry energy from heavy ion collision at intermediate energy.

Projectile fragmentation is very useful for producing radioactive ion beams. A model for projectile fragmentation is developed which involves traditional concepts of heavy-ion reaction (abrasion) plus the well known statistical model of multifragmentation (Canonical Thermodynamical Model) and evaporation. A very simple impact parameter dependence of freeze-out temperature is incorporated in the model which helps to analyze the more peripheral collisions. The initial conditions of projectile fragmentation are also determined from transport model calculation based on Boltzmann-Uehling-Uhlenbeck (BUU) equation and compared with the used parametrization. The projectile fragmentation model is successfully applied to calculate the production cross-sections for a wide range of exotic as well as stable nuclei of different projectile fragmentation reactions at different energies. Different important observables of projectile fragmentation like intermediate mass fragments, largest cluster size, differential charge distribution etc are also calculated from this model and compared with experimental data. A hybrid model is also developed separately for explaining multifragmentation reaction reaction around Fermi energy domain.

The underlying physical assumption behind canonical and grand canonical models is fundamentally different, and in principle agrees only in the thermodynamical limit when the number of particles becomes infinite. Nevertheless, we show that these models are equivalent in the sense that they predict similar results if certain conditions are met even for finite nuclei. An analytical formula is derived which enables one to extract canonical results from a grand canonical calculation and vice versa.

Study of nuclear symmetry energy in intermediate energy heavy ion reactions is an important area of research for determining the nuclear equation of state. In this thesis, symmetry energy coefficient is determined by different ways (isoscaling source method, isoscaling fragment method, fluctuation method and isobaric yield ratio method) in the framework of canonical and grand canonical models. We have also studied, how the secondary decay from excited states affects and observed that the best possible way to deduce the value of the symmetry energy is to use the fragment yield at the breakup stage of the reaction (not the "cold" fragments).

Another important area in the study of intermediate energy heavy ion collisions is the phenomenon of phase coexistence or liquid gas phase transition. The standard methods of theoretical studies on liquid-gas phase transition at intermediate energy collisions assume that because of two body collisions nucleons equilibrate in a given volume and then dissociate into composites of different sizes according to availability of phase space. This thesis focuses on whether results of transport model calculations (BUU) at intermediate energy can point to signatures of phase transition. To do that, a simplified yet accurate method of transport model is developed which allows calculation of fluctuations in systems much larger than what was considered feasible in a well-known and already existing model. The distribution of clusters is remarkably similar to that obtained in equilibrium statistical model and provides evidence of phase transition.

The focus of my thesis was to explore and understand the mechanisms of particle production at intermediate transverse momenta (pT) , 2< pT < 5 GeV/c, in ultra-relativistic heavy ion collisions where a strongly interaction medium of deconfined quarks and gluons , the quark gluon plasma (QGP) is produced. An unusually enhanced production of baryons over mesons from these collisions, reported for the first time at the RHIC (Relativistic Heavy Ion Colliders) heavy ion programme, had not been predicted earlier by any of the established models of particle production. A succinct explanation to the observed “baryon anomaly” was offered by the models invoking hadronization by recombination or coalescence of quarks. The constituent quark number (ncq) scaling of the elliptic flow coefficients, v2, of different particle-species was also a suggestive of coalescence being a plausible mechanism of hadronization at these pT range.

Since then a lot of theoretical investigations were pursued to unveil the enigma of particle production particularly in the region of “baryon anomaly”. In my thesis work, I have adopted the technique of two-particle angular correlations to probe whether the strength of correlation is sensitive to the mechanisms of particular production. To quantify the effect, the near side jet-like yield associated with baryon-hadron and meson-hadron angular correlations were calculated. Baryon production being favoured within the coalescence formalism, a naive expectation would be, a suppressed baryon triggered jet-like yield (trigger dilution) as it is unlikely to have correlated partners at small angle. I have explicitly look for this signature in data and Monte Carlo event generators that implement coalescence as a mode of hadronization.

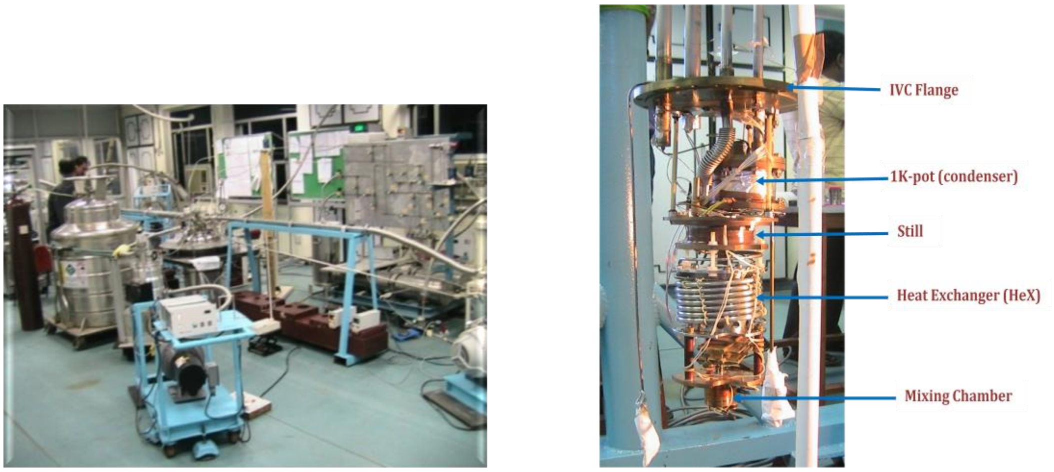
The two particle angular correlation measurements between leading particles (trigger), identified as mesons (pion) or baryons (proton/anti-protons), and unidentified charged hadrons (associated) was performed on the data recorded by A Large Ion Collider Experiment (ALICE) at the CERNs' Large Hadron Collider (LHC) in Pb-Pb collisions at 2.76 TeV. Pure samples of pions and (anti-)protons were obtained on a track-by-track basis through a combined nσ PID method using the specific energy loss (dE/dx) information from the ALICE-Time Projection Chamber (TPC) and the timing information from the ALICE-Time of Flight (TOF) detectors.

The near side per-trigger jet yields were calculated as a function of collision centrality, expressed in terms of number of participating nucleons, Npart. Both pion and proton triggered jet yields increase with centrality however; the rate of increase has a trigger species dependence. The associated near side yield for pion triggered correlations increase smoothly with the centrality. The proton triggered yields are however, systematically lower than the pion triggered yields but it also rises marginally with Npart and saturates. Interestingly, within the error bar, baryon triggered yield at the most central and peripheral collisions are of similar magnitudes. In contrary, pion triggered yield exhibits almost a liner increase as function of collision centrality.

The enhancement of jet-like yield associated with pion or unidentified charged hadrons may be attributed to the jet-quenching and/or medium-induced modification of jet fragmentation functions. On the other hand, the observed suppression (or lack-of enhancement) for non-pion or baryon triggers might be interpreted as a combined effect of competing processes that involve jet-medium interactions (jet quenching) and quark recombination. If particles are dominantly produced from the recombination of boosted thermal quarks, suppression in the per-trigger yield could be naturally expected, because hadrons produced from the recombination of thermal partons are unlikely to have jet-like correlated partners in small angles. This suppression would be stronger for baryons as baryons are dominantly produced from such a mechanism over mesons. The initial rise in case of proton triggered correlation could be an effect of modified jet fragmentation in a color charged medium. This could be a dominant effect in mid-central or peripheral collisions. But, with the increase in centrality, the effect of quark-recombination takes over and more baryons are produced without associated hadrons. The combined effect of these two competing processes results in the saturation of the baryon-triggered yield. Therefore, this thesis provides relevant information on the nature of particle production and microscopic processes that drive baryon-to-meson enhancement.

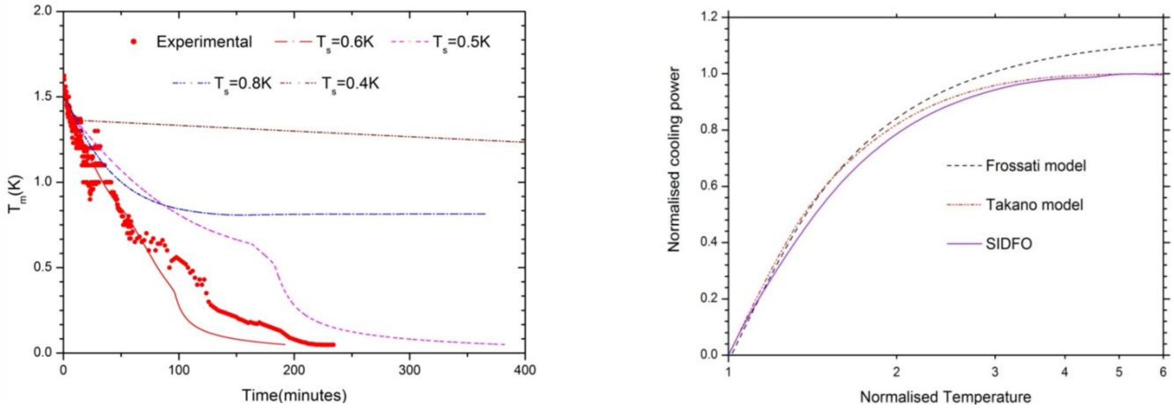
A thermal model of dilution refrigerator is formulated using numerical simulation program SIDFO (Simulation of Integrated Dilution refrigerator For Optimization). It can simulate varying process parameters and can be used for calculations prior to any process modifications. In addition it allowed us to carry out a comprehensive study of time dependent analysis of transitory phase. Furthermore, with this approach new process equipments can be easily added.

While many analyses and models of the thermo-dynamical process related to dilution refrigerator already exist, the present work describes the congregation of all components of the dilution refrigerator making up a complete closed cycle simulation. The simulation is further upgraded to accommodate the stages of development preceding the steady state condition by introducing time dependent variations.



(a) (b)

Fig. 1.4.1(a) Dilution refrigerator set-up developed in the laboratory, (b) Dilutions insert showing different components which are designed using SIDFO and fabricated.



(a) (b)

Fig. 1.4.2(a) Dilution refrigerator was successfully cool-down below 50mK along with the calculated SIDFO results under four different STILL temperatures/heaters, (b) Comparisons of cooling power of dilution refrigerator with other existing models.

To the best of knowledge, no comprehensive study to investigate the time dependent manifestation of transitory phases in dilution refrigerator has been done earlier. Moreover, simulation has produced several unique results of the underlying phenomena occurring at various stages of the low temperature process. Thermo dynamical analysis of steady state and transient processes through SIDFO has helped to conceptualize and design a complete dilution refrigeration system. The dilution refrigerator was successfully built and temperature down to below 50mK have been achieved and maintained for hours. The results of simulation as well as results based on other existing models are compared with experimental data derived from measurements.

One of the important aspects in nuclear many body system has been to describe the emergence of collective features of nuclei as well as their structure in terms of the individual motion of nucleons. Giant dipole resonance (GDR), the most prominent collective mode of excitation, present in all nuclei, has been studied extensively and considered as an important tool to probe the properties of atomic nuclei at the extreme conditions of spin and temperature. The GDR can be understood macroscopically as the out-of-phase oscillation between the protons and neutrons, and microscopically in terms of coherent particle-hole excitations. The GDR decays via high energy γ-ray emission (10-25 MeV) which occurs at early stage of compound nuclear decay and competes with the particle emission. The high energy gamma-rays are the cleanest probe to study GDR properties as the gamma rays are not strongly affected by the nuclear medium. The decaying gamma- rays from the GDR vibration of nuclei have the characteristics of Lorentzian strength function. The centroid energy of this strength function is related to the nuclear symmetry energy which is useful for the investigation of equation of state in nuclear matter and also has astrophysical interest. Interestingly, the GDR also couples with the nuclear shape degrees of freedom and therefore can directly probe the nuclear deformation. Along with that, the time scale of GDR vibration is very short and thus provides valuable information in different interesting nuclear phenomena like loss of collectivity, neutron-proton asymmetry at high temperatures, angular momentum driven exotics shapes, Jacobi shape transition at very high spins, superdeformation of the alpha-cluster nuclei, etc.

The primary interest in GDR research lies in the understanding of the GDR width of hot and rapidly rotating nuclei, as it is the major source of information on nuclear damping and shape evolution at extreme conditions. The experimental studies on the evolution of GDR width, over the years, have shown that the GDR width increases with both temperature (T) and angular momentum (J), whereas its centroid energy remains mostly unchanged as T and J vary. In this regard, it is worthwhile to mention that the effect of J and T on the GDR width becomes noticeable only above a critical angular momentum, $J_c \sim 0.6A^{5/6}$ and $T \sim 1$ MeV. Although, a wealth of data exists on the angular momentum dependence of GDR width in different mass regions, the measurement of the GDR width at low temperatures (T < 1 MeV) is rather scarce due to the experimental difficulties in populating the nuclei at low excitation energies. This work presents a systematic as well as precise experimental data to investigate the influence of GDR induced quadrupole moment on GDR width, in the unexplored temperature range T=0.8-1.5 MeV, for the first time, in $A \sim 100$ mass region. It is also our endeavour to systematically assess the different theoretical models and understand the complete nature of the damping mechanism as a function of T inside the atomic nucleus.

The experiments were performed using the alpha beam from K-130 cyclotron at the Variable Energy Cyclotron Centre (VECC), Kolkata, India. A self-supporting 1 mg/cm^2 thick ^{93}Nb target was bombarded with the alpha beams produced by the K-130 cyclotron at four different incident energies of 28, 35, 42 and 50 MeV to populate the compound nucleus 97Tc at the excitation energies of 29.3, 36.0, 43.0 and 50.4 MeV, respectively. The high-energy gamma-rays from the GDR decay were measured using the Large Area Modular BaF_2 Detector Array (LAMBDA-consists of 49 BaF_2 detector arranged in 7×7 matrix). A 50 element low energy γ-multiplicity filter (consisting of 50 BaF_2 detectors arranged in two 5×5 array, placed at top and bottom of the scattering chamber) was used to estimate the angular momentum populated in the compound nucleus (CN) as well as to get a fast start trigger for time-of-flight (TOF) measurement. In addition, a liquid scintillator based neutron detector was also used to obtain the nuclear level density parameter (which is an important input in the statistical model calculation) by measuring the evaporated neutron energy spectra. The TOF technique was used to separate the neutron background in the high-energy gamma spectrum while pile up events were rejected using the pulse shape discrimination (PSD) technique. The high energy γ-ray spectra were extracted by gating on different folds of the multiplicity events from the offline analysis of the data recorded in event-by-event mode by applying all the necessary cuts and rejections. The fold gated high energy gamma-rays spectra are compared with the statistical model calculation (CASCADE) to extract the GDR parameters at different temperature and angular momentum.

Interestingly, it has been observed that the experimental GDR width remains nearly constant at the ground state value up to T ~ 1 MeV and increases thereafter.

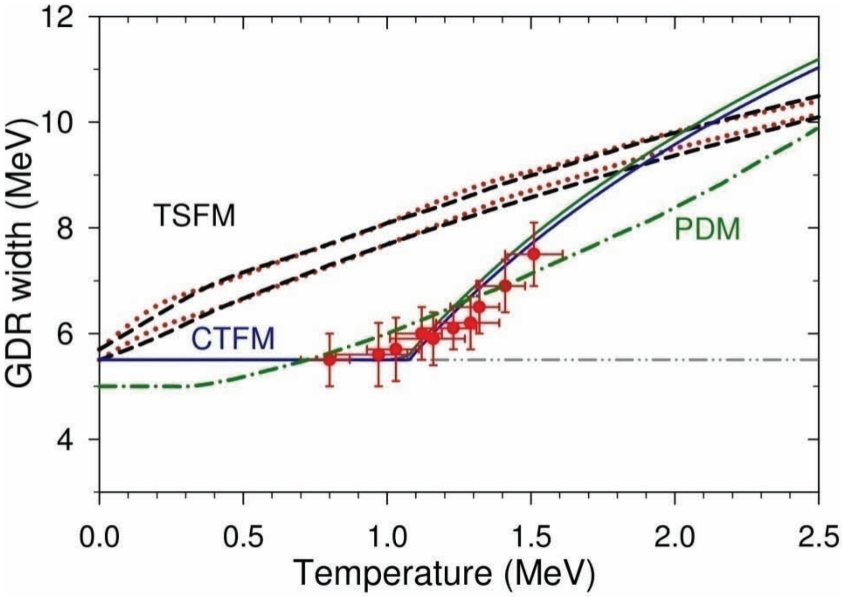


Figure 1.4.3.: GDR width as a function of temperature compared with macroscopic (TSFM and CTFM) and microscopic (PDM) theoretical calculations. The red dotted line represents the TSFM with shell effect and black dashed line represents the TSFM without shell effect. TSFM and CTFM are shown for two sets of angular momentum (J = 10 and 20 h)

The measured GDR widths at very low temperatures (T=0.8 - 1.5 MeV) were compared with the different theoretical calculations of GDR width such as macroscopic Thermal Shape Fluctuation Model (TSFM), phenomenological Critical Temperature Fluctuation Model (CTFM) and microscopic Phonon Damping Model (PDM). The TSFM is based on the large-amplitude thermal fluctuations of the nuclear shape under the assumption (adiabatic assumption) that the time scale associated with thermal fluctuations is slow compared to GDR vibrations. In TSFM, the GDR strength function is calculated by averaging the line shapes corresponding to the different possible deformations of the nuclear shape. The phenomenological CTFM model is based on the the competition between GDR induced intrinsic fluctuation and thermal shape fluctuation at low temperatures. On the otherhand, in the microscopic PDM calculation, the GDR damping mechanism is caused by coupling of the GDR to non-collective particle-hole (ph) and particle-particle (pp) [hole-hole (hh)] configurations. Interestingly, it has been observed that the microscopic PDM and phenomenological CTFM describe the data reasonably well, whereas the adiabatic TSFM differs substantially even after inclusion of shell effect. This interesting result clearly suggests that the suppression of the GDR width at these low T is a general feature for all nuclei and cannot be explained including only shell effects. The present results also indicate that the effect of GDR induced intrinsic fluctuation could be one of the ways in explaining macroscopically the behaviour of GDR width at low T. However, this effect is not explicitly needed in microscopic PDM, rather thermal pairing should be included to have adequate description of the damping of GDR width at low T. Nevertheless, the present experimental study does provide a stringent testing ground of the theoretical models on the damping mechanism of collective vibration inside the atomic nuclei.

It is widely believed that primordial matter that was existent at the earliest stages of the creation of the Universe, less than a few microseconds after the Big Bang can be created experimentally in relativistic heavy ion collisions under extreme conditions of temperature and energy density. The Relativistic Heavy Ion Collider (RHIC) at BNL, USA has undertaken heavy-ion, proton-proton and proton-ion collisions for the past 15 years to create and investigate the new phase of de-confined matter commonly referred to as the Quark Gluon Plasma (QGP). This new state of strongly interacting matter is characterized by asymptotically free quarks and gluons. The measurements at RHIC over the last few years have set forward conclusive evidences towards the formation of QGP. The STAR (Solenoidal Tracker at RHIC) experiment at RHIC is designed to search for the existence of the QGP and to explore its properties. Experimentally, this new state of matter is studied via the detection of the products of heavy-ion collisions. Suitable observables constructed from the different properties of the particles detected are used to understand the underlying mechanisms. This thesis work is mainly aimed at probing the matter created at RHIC heavy-ion collisions using di-muons and photons at mid and forward rapidities. This work is partly focused on fabricating and testing Multi-gap Resistive Plate Chambers (MRPC) for the Muon Telescope Detector (MTD) upgrade of the STAR experiment at mid-rapidity, whose objective is to detect muons using excellent timing and position resolution of the MRPC's. This thesis work has also emphasized on studying the correlation between charged particles and photons measured in the common η- phase space of the two forward detectors at STAR, the Forward Time Projection Chamber (FTPC) and the Photon Multiplicity Detector (PMD), respectively, at a wide range of Au+Au collision energies. This work is performed to search for possible evidences of the QCD chiral phase transition from the QGP phase to the Hadronic Gas (HG) phase.

Fabrication and testing of Multi-gap Resistive Plate Chambers (MRPC) for the STAR-MTD project:

The Muon Telescope Detector (MTD) installed at mid-rapidity at STAR wishes to probe the new state of matter created in RHIC by studying the di-muon spectra at different mass regimes. Data taken by the MTD detector will help the scientific community to understand the elementary properties of the QGP such as the temperature and color screeningaspects. The MTD is capable of providing excellent muon identification and trigger capabilities in the high-luminosity eraat RHIC. In order to meet the desired physics goals, the MTD relies on clean muon identification and triggering using precise timing and hit position measurement and hence uses the inexpensive and reliable MRPC technology, well known for its excellent timing and spatial resolution. As a part of my thesis work, 10 MTD-MRPC modules of dimensions 87 cm x 58 cm and five 250 μm gas gaps,have been fabricated and tested successfully at VECC. The 10 modules constitute ~10% of the modules installed at STAR. The modules weretested in the avalanche mode with a gas mixture of Freon and Iso-butane in the ratio 95 : 5. The modules havedouble-ended, 3.8 cm wide readout PCB pads with 0.6 cm gaps in between. I have been involved in the testingand characterization, including detector seasoning, data taking on efficiency, noise rate, charge spectra and timingresolution measurement of all the modules. A timing resolution <100 ps and a spatial resolution of ~1 cm, which are suitable for ourphysics goals have been measured in cosmic ray tests and with test beams.

Charged-neutral (γ) correlation analysis for the STAR experiment:

The phase transition from QGP to Hadron Gas is associated with the de-confinement and the chiral phase transitions. When the system passes through a chiral phase transition, there could be formation of metastable domains of disoriented chiral condensate (DCC). Formation and decay of DCC domains will lead to anti-correlation of charged and neutral particle multiplicities. We have measured the correlations between photons and charged particle multiplicities in the pseudo-rapidity range $-3.7 < \eta < -2.8$ using the PMD and the FTPC detectors, in Au + Au collisions, to search for possible signals of anti-correlation. This measurement has been done for the RHIC Beam Energy Scan (BES) program over an energy range of 19.6 to 200 GeV. The analysis has been performed in the ROOT framework of the STAR computing environment. As a part of this analysis work, I have performed extensive cleanup of the datasets, error analysis and model calculations. For the top RHIC energy (200 GeV), we have observed a non-zero signal of dynamical fluctuation beyond model predictions only when the photons and the charged particles are measured in the same acceptance. The observables for the correlation analysis were developed and tested on the models representing heavy-ion data at RHIC. The data has been compared with non-DCC models and within systematic uncertainties we have observed ~1% deviation from baseline prediction.

Use of MRPC for TOF-PET (Time-of-Flight Positron Emission Tomography):-

As a spin-off benefit of the Detector development for STAR, I have done parallel R&D with similar detectors (MRPC), for medical applications. MRPC, because of its excellent time resolution is considered to be apotential candidate for TOF-PET systems. In order to explore this avenue, I have built several glass-based, smallsized (16 cm x 10 cm, 16.5 cm x 16.5 cm) MRPC's and have setup a system to detect 511 keV photon pairs froma ^{22}Na source. The pair of anti-parallel 511 keV photons emitted by the source created via positron-electron annihilation have been detected by a coincidence set-up of the 6-gap MRPC and a plastic scintillator of 5 cm x 1.2 cm dimensions. The measurement has been performed with source and non-source configurations to remove cosmic muon background. The contribution due to the source was clearly distinguishable by the detection of photon pairs above background. A photon detection efficiency of 0.9% is obtained at the operating voltage of the MRPC. An effort was made to locate the position of the source using coincident timing distribution measurement of the MRPC and the scintillator and comparing the value obtained with simple calculations using known distances and the photon velocity. Given the large error bars in the measurement, the measured and calculated values showed a similar trend.

The Superconducting Magnetic Energy Storage (SMES) is a contemporary field of research having promising solutions for achieving high quality power that is required for many applications including accelerators. This thesis deals with design and optimization of superconducting magnet system for energy storage application. There are several design issues of a SMES magnet, including the amount of stored energy, operating temperature, operating current, cooling method, operating cost, conductor stability against fast field-transients, *etc.* The essential basis of the design is the critical characteristics of the particular superconductor at the operating temperature. The thesis consists of two parts: The first part describes the design, development and test results of a 0.6 MJ solenoid-type SMES system integrated with power-conditioning system; The second part describes design of two different configurations (solenoid-type and sector toroid-type) of a 4.5-5.0 MJ SMES system, where a novel approach of design optimization based on Differential Evolution algorithm has been adopted. A liquid helium bath cooled 0.6 MJ SMES system using cryostable conductor, integrated with the power-conditioning system, has been designed, developed and tested for carrying out research on the interaction between SMES and electrical power system. The thesis-work includes a detailed magneto-structural analysis of the system to determine minimum winding tension that ensures radial compressive stress of the coil in all possible scenarios. Various parameters of the magnet coil have been optimized to maximize the stored energy and minimize the capital cost in terms of conductor length. Finally, the system is connected to the load through the power conditioning unit and voltage sag compensation of various magnitudes is demonstrated.

In the second part, work is pursued to establish the correlation of geometrical parameter and develop optimization approach to design and understand superconducting magnet parameters for energy storage application. Unlike previous published papers, this work gives an analytical formulation of the optimization problem in terms of coil parameters and aims to minimize cryogenic refrigeration load into the cryostat using differential evolution (DE) algorithm, which in turn reduces the operating cost of the system. The corresponding optimal design of 5MJ class SMES coil using Rutherford-type cable is discussed as a case study. Effect of allowable hoop stress in the winding and maximum allowable voltage across the coil to the refrigeration load and coil parameters are also been investigated. As a consequence of low magnetic stray field, further, a multi-objective optimization design approach for sector toroidal superconducting magnetic energy storage coil has been developed considering the practical engineering constraints. The objectives include the minimization of necessary superconductor length and torus overall size, which determines a significant part of cost towards realization of SMES. Unlike the single objective optimization, the solution of multi-objective optimization problem is not a single point, but a set of nondominated points known as Pareto optimal solution. The best trade-off between the necessary conductor length for winding and magnet overall size for different number of sector coils is achieved in the Pareto-optimal solutions, the compact magnet size leads to increase in required superconducting cable length or vice versa. The final choice among Pareto optimal configurations and number of sectors is made in relation to other issues such as ac loss during transient operation, stray magnetic field at outside the coil assembly, available discharge period, etc.

The best feasible Pareto solution for the 4.5MJ/1MW system is determined (*major radius*=0.62-0.67 m) considering the practical engineering aspects without losing the optimality. The proposed design approach is adapted for a 4.5 MJ/1MW SEMES system using low temperature niobium-titanium based Rutherford type cable. Furthermore, the validity of the representative Pareto solutions is confirmed by finite-element analysis (FEA) with a reasonably acceptable accuracy.

Magnetic field transient analysis has also been carried out to evaluate transient loss and assess the feasibility of using helium re-condensation technology with commercially available cryo-refrigerators. The total transient loss comprising from both AC loss from superconductor and eddy loss from coil former with support structure would be around 1000 J at 4.2 K (considering about 25 % contingency) and must be handled by cryogenics system. This energy is equivalent to boil-off of 0.4 litre of liquid helium. If the discharge occurs eight times a day, this provides an additional heat load of 2% to the steady state heat load. The steady state load to the helium chamber is calculated to be around 2.0 W at 4.2 K. It is proposed to have three numbers of two-stage Gifford-McMahon (GM) type cryo-refrigerator (1.5 W at 4.2 K each) to mitigate both transient and steady state load. The total heat load combining both steady state and transient load in the intermediate thermal shield made of copper around the liquid helium system is around 180 W at 60 K, which is well within the capacity of a standard commercially available single-stage cryo-refrigerator. In adiabatic situation, the maximum temperature rise of thermal shield during transient of 200A/s (1.2 T/s) is found to be less than 0.3 K. The mechanical von-Mises stress developed on the intermediate shield due to interaction of induced current density and magnetic field for maximum field transients is found to be around 6.2 MPa, which suggest that the thermal shield would be safe from any structural deformation during field transient. Finally, quench protection scenario has also been investigated suitable for this toroidal-type SMES system. A viable electrical connection scheme for quench protection is developed. Heater induced active quench protection in fail-safe mode is found to be better option for quench protection ensuring no magnet damage.

1.5 Saha Institute of Nuclear Physics (SINP), Kolkata

Ten students completed doctoral programme in Physical Sciences during this period and Ph.D. degrees were awarded. A break-up of subject areas a of theses are A) Cosmology, B) Relativistic Heavy Ion Physics, C) Experimental Condensed Matter Physics, D) Astroparticle Physics, E) Plasma Physics and F) Experimental Atomic Physics. Main findings of these theses are the following.

A) Cosmology:

Atanu Kumar in his thesis titled ‘Evolution of Cosmological Perturbations through bounce in covariant perturbation thoery and tests of lineariry’ studied some characteristics of bouncing cosmology and emergence of scale invariant spectrum from a bounce. This was carried out by setting up some conditions for linearity of perturbations and the evolution of cosmological perturbations was investigated through a simple toy model for bounce.

B) Relativistic Heavy Ion Physics:

The thesis titled ‘Study of hot and dense nuclear matter in effective QCD model’ by Chaudhuri Aminul Islam focused on the study of properties of Quark Gluon Plasma (QGP) in the NJL, PNJL, EPNJL and Color Singlet models. He investigated the correlation function (CF) and spectral properties associated with it using QCD models because hadronic properties are embedded in CFs.

C) Experimental Condensed Matter Physics:

Susmita Dhara studied the changes of magnetic and transport properties of CO_xCu_(1-x) granular alloys with the variation of Co concentration in her thesis. Co-rich core favoured ferromagnetism whereas the shell with less Co supported superparamagnetic behaviour. Spin glass type behaviour was found in annealed samples. New results were obtained in relaxation measurements.

D) Astroparticle Physics:

The thesis of Apurba Kheto discussed the effect of entrainment in superfluid neutron star matter and its application to rotating neutron stars. This was studied in the two fluid model adopting a relativistic field theoretical model for baryon-baryon interaction mediated by mesons. The author showed that the entrainment parameter was strongly enhanced due to the isospin effect. Later the influence of entrainment on the properties of rotating neutron stars was reported in the thesis. Kamaksha Prasad Modak explored some aspects of Dark Matter indirect detection using various Dark Matter particle physics models in his thesis. He investigated this problem in the scalar singlet DM model, the inert Higgs doublet DM model and the two component scalar DM model. The observational data on the annihilation products of Dark Matter in the Galactic Centre, Galaxy Clusters and extra-galactic sources were explained based on those models. The thesis of Prasanta Char focused on the impact of strange matter equation of state (EoS) involving hyperons and Bose-Einstein condensates of antikaons on core collapse supernova (CCSN) simulations and structures of neutron stars. He demonstrated that the newly constructed equations of state were compatible with the observed two solar mass neutron stars. It was also noted that the protoneutron star evolved to a stable neutron star in the long duration CCSN simulation using the hyperon EoS which has important implications for SN1987A. He also reported his work on magneto-elastic oscillations of neutron stars in the thesis. Amit Datta Banik studied the phenomenology of Dark Matter (DM) and the extension of the Standard Model to this issue. He explored the minimal fermionic dark matter in two Higgs doublet model and tested viability of the model with experimental bounds. This was followed by a detailed study of Inert Doublet Model with an additional scalar singlet. Interesting features of the model involving Higgs to diphoton decay were found. Furthermore, he proposed a model for hidden sector fermionic dark matter and investigated throughly dark matter annihilation in this model in order to explain the updated Galactic Centre gamma ray flux along with the dwarf galaxy gamma ray observations.

E) Plasma Physics:

Abhik Mukherjee presented his research work on the theory of tsunami wave and rogue wave propagations in shallow and deep waters and their applications to practical problems in the thesis. He made significant contributions in theory of non-linear wave propagation. The thesis of Sourav Pramanik dealt with the theoretical treatment of the dynamics of a cold electron beam moving between two electrodes in a planar diode. He investigated the impact of a transverse magnetic field on the space charge limited current as well as aperiodic instabilities. New and interesting results were presented here.

F) Experimental Atomic Physics:

Hitesh V. Rahangdale described the experimental investigation of strongly bound L-shell ionization of high -Z atoms under the influence of 16-45 KeV electrons in his thesis. A new experimental facility was developed for this study. The analysis of data was carried out using simulations of the electron beam trajectory in the films with Monte Carlo codes.

1.6 Institute of Physics (IOP), Bhubaneswar

At the Institute of Physics, the work is carried out in the areas of theoretical and experimental condensed matter physics, high energy physics, and nuclear physics. Three Ph.D. degrees were awarded in theoretical physics and two were in experimental physics. In the case of each dissertation, many pieces of work were carried out. Below, a selection of research work done in each case is presented.

A. Experimental Physics

Nanostructures have been studied for the semiconductors ZnO and GeO_2. The main goal was to find a simple single step growth techniques for variable oxygen deficient Au capped ZnO and GeO_2 hetero-nanostructures (Hns) of various morphologies and dimensionalities. Enhanced field emission and visible-light driven properties of these samples were studied. Growth mechanisms of various morphologies have been proposed.

Nano-patterns on single crystal semiconducting rutile TiO_2 surfaces and metallic Tantalum surfaces via the technique of ion irradiation were generated. In both cases nanostructures were generated through the competition between the erosion and diffusion processes. The scaling studies on these non-equilibrium surfaces as well as the scaling exponents showed that these surfaces belong to different universal classes. Results further showed that the inclusion of Schwoebel barrier in the metallic tantalum was important for understanding pattern formation. On the TiO_2(110) surface, preferential sputtering of oxygen atoms leads to the formation of Ti rich zones that become the nucleation sites for the development of nanostructures. The results show an enhanced photoabsorption from these nano-patterned surfaces. Development of nanostructures on the surface and creation of vacancy sites along

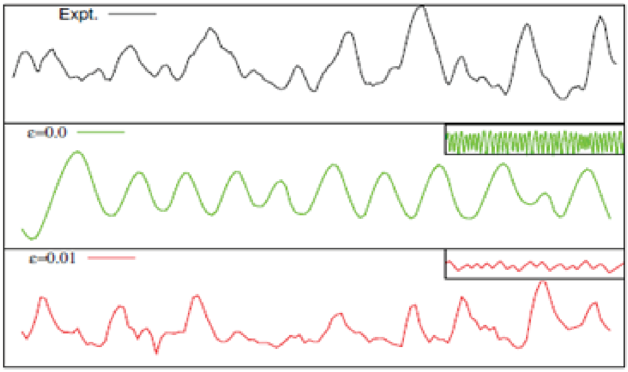


Figure 1.6.1. Comparison of surface profile (h(x,t)) of experiment with the simulations. The simulated profiles were obtained by KMC model with the parameters p=0.1, Jc/kBT = 0.25 and e=0.0 or 0.01. Inset shows the steady state profile of the surface

.with the formation of $Ti_{1-x}Co_xO_2$, CoT iO_3 and Co nanoclusters, upon ion irradiation, promote the high photoabsorption and the reduced band gaps observed here. Formation of the cobalt nanoclusters, after implantation, also displays anisotropic superparamagnetic properties in this system. Scaling studies above blocking temperature also display this anisotropy. Presence of nanoclusters, with dipole-dipole interactions and inter-cluster exchange interactions, produce these anisotropies. RBS/C results also display presence of these Cobalt-clusters along with an increase in depth dependent damage below the surface. Multiple scattering formalism has been applied to obtain the depth dependent damage profiles which indicate dynamical annealing of defects at the End-of-range. Scaling studies of TiO2 surfaces, based on the non equilibrium growth models, indicate that these surfaces after irradiation belong to the EW class. In the nanopatterns created on the metallic Tantalum surfaces, Schwoebel barrier plays an important role as has been demonstrated here through 1+1 dimensional KMC simulations. The Schwoebel effect has been incorporated here via a weak non linearity in the Hamiltonian. Comparison of simulations with experimental results show that the morphology of ion irradiated Tantalum surfaces, as shown in figure, belongs to a universality class other than EW and KPZ.

B. Theoretical Physics

DNA when suspended in a solvent separates completely in two strands at critical temperature. It undergoes second-order phase transition. Elastic response of the double-strand DNA and Efimov DNA near critical temperature was studied. Three different models of DNA were used. Phase diagrams were obtained. In one of the model, the nature of transition changes to first-order.

Two important phase transitions associated with QCD, namely chiral symmetry breaking transition and confinement-deconfinement transition were studied employing the techniques of reaction-diffusion equations. It was shown that well-defined traveling front solutions, mimicking phase boundaries for a first-order transition, exist though the relevant QCD transitions are of second-order or a cross-over. So long as dissipation dominates, a transition proceeds by a slow-moving front and a long-lasting mixed phase state prevails in the several fm time it takes to complete the transition. This is expected to leave its stamp on the various signals of QGP. Possibility of formation of disoriented chiral condensates (DCC) in high multiplicity pp collisions at LHC energy has also been explored. It is argued that boundary conditions necessary for the existence of slowly propagating front solutions of reaction-diffusion equations ensure that a large DCC domain is produced. The decay of the DCC domain can lead to relatively clean signals of coherent pion emission.

Quantum entanglement and Quantum Correlations that go beyond Entanglement (QcbE) are considered. Till date there exist no unique characterization method for quantum entanglement and QCbE in multiparticle systems. A detection method of entanglement in higher dimensional systems using the modified form of quantum co-variance has been proposed. It is argued that quantum discord may capture local as well as nonlocal quantumness. Here, by local quantumness we mean local superposition (single particle) in a system of more than one particles. If this superposition can be masked by writing down the state in a different decomposition --- then the state has no local quantumness in it. The nonlocal superposition is the superposition of the states of two or more particles. The notion of quantum discord is generalized using multivariate mutual information, to characterize the quantum properties of a multiparticle system. This new measure, called dissension, is a set of numbers -- quantumness vector. It is studied for multi-qubit systems, particularly for three qubits and four qubits.

To give physical meaning to quantum correlations, some tasks are considered. The concurrence monotones are used to develop some hierarchy of inequality relations by which one can infer whether a two-qudit state is useful for teleportation. A swapping network is considered. The results show that the entanglement between nodes of the network determines how much classical and quantum information one can send. It is shown that using any kind of local and nonlocal universal or state dependent cloning machines, the optimal broadcasting of QCbE is impossible indicating that the entanglement and QCbE are two distinct quantities. It is also shown that the better we clone (delete) a state, the more difficult it will be to bring the state back to its original form by the process of deleting (cloning).

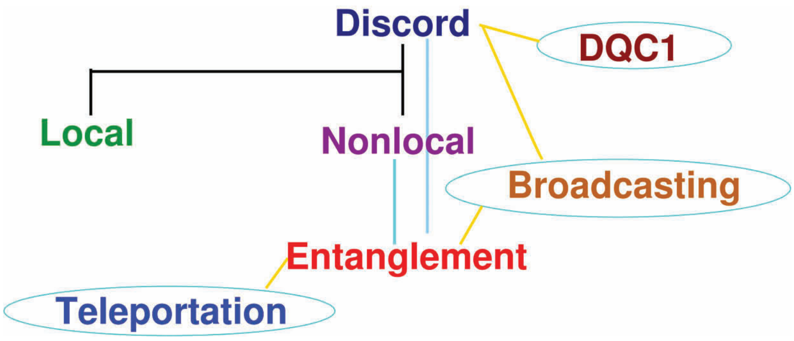


Fig. 1.6.2: *The light blue line represents the hierarchy, cyan the equivalence, yellow the application and black lines the types. Entanglement is always stronger than discord.*

1.7 Harish-Chandra Research Institute (HRI), Allahabad

During the period, 7 students were awarded Ph.D. degree in Physical Sciences. Highlights from some the theses are presented as follows.

Finer Consistency Checks on BPS Black Hole Entropy in String Theory revolves around the central theme of black hole entropy matching, widening its scope and applicability to further reinforce the internal consistency of string theory. The thesis consists of two original works each fitting broadly under the encompassing framework of black hole microstate & macrostate counting within string theory. We attempted to give a physical explanation behind a set of ad hoc rules necessary to match the microscopic counting to the entropy of $\frac{1}{4}$BPS black holes in N = 4 string theory. In a later work, we precisely reproduced certain logarithmic terms emerging from the large charge expansion of twisted microscopic indices from respective quantum corrections to $\frac{1}{4}$BPS &$\frac{1}{8}$BPS black holes in N = 4 &N =8 supergravity theories.

Avinanda Chaudhuri discovered some important links between seesaw mechanisms of neutrino mass generation and other aspects of new physics in the world of elementary particles. First, she demonstrated that the Type-II seesaw mechanism can be consistent with a predictive form of the neutrino mass matrix, name, texture zero mass matrices, only if there are at least two scalar triplets. Subsequently she established connections between such situations and observations that can be made at the Large Hadron Collider. Her other contribution was to develop a model of Dark Matter (DM) of the universe by extending the Type-III seesaw mechanism. She found that such theoretical models predicted the DM particle mass in some specific ranges only.

In her thesis Akansha Singh dealt with the problem of surface supported clusters that is relevant for a number of applications including sensing, formation of self-assembled nano-structures, nano-electronics and heterogeneous catalysis. Three major findings of Akansha's work are the following.

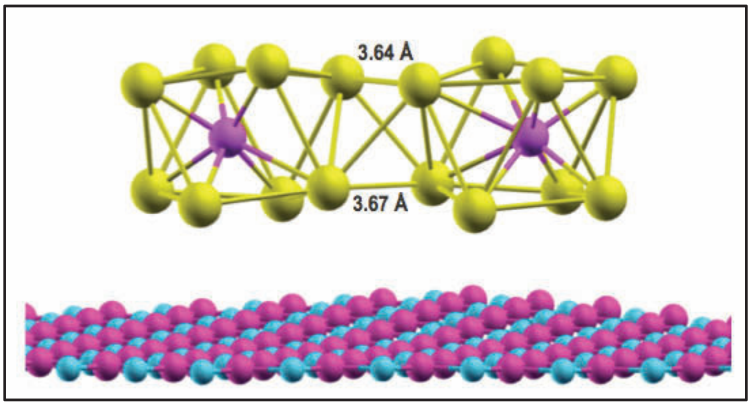


Figure 1.7.1. FeCa$_8$ dimer on a h-BN substrate.

Few-atom silver clusters, when deposited on a stepped graphite surface, interact strongly with the step edges, dissociate into individual atoms which diffuse towards the edges. Once at the edge, the silver atoms tend to align along the edge to form self-assembled metallic nano-wires.

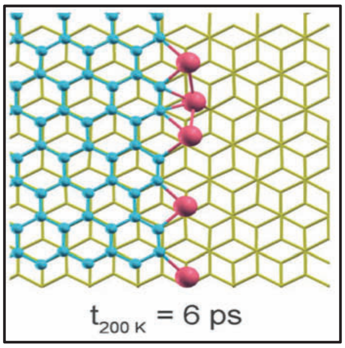


Figure 1.7.2. Self-assembled silver nano-wire at a step edge on graphite surface.

Individual FaC$_8$ magnetic superatoms retain their intrinsic properties on graphene and hexagonal BN substrates. They can form self-assembly on h-BN substrate once the density crosses ~ 12 × 10^{13}/cm^2. An Ag$_2$Au cluster supported on an alumina substrate is a promising catalyst for CO oxidation reaction, although the isolated Ag$_2$Au cluster is not. The kinetic barrier to O$_2$ dissociation is estimated to be less than an eV for the supported cluster.

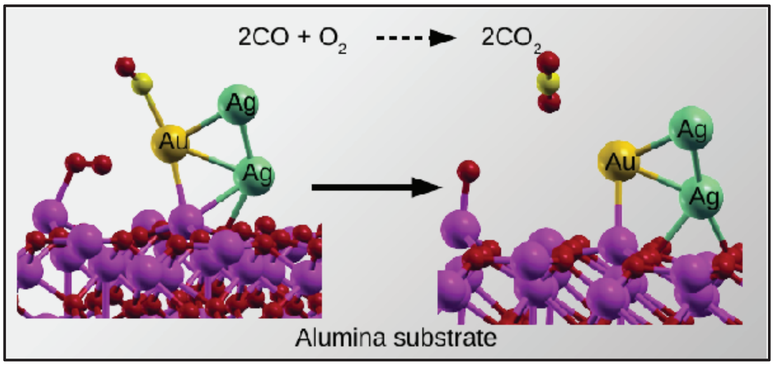


Figure 1.7.3. CO oxidation catalyzed by an Ag_2Au cluster on alumina substrate.

Quantum correlations present in shared systems are known to be crucial for several quantum information-theoretic protocols that are either not possible in the classical domain or possible with a reduced efficiency. The practical availability of these protocols in quantum devices, however, strongly depends on the survival of quantum correlations when the underlying system is exposed to the external environment. Therefore, it is important to study the stability of quantum correlations in systems composed of several particles in the presence of environmental effects. In the present dissertation, we have studied the survival of bipartite and multipartite entanglement in many-particle quantum systems under various forms of external effects.

In some cases, these external effects have been modelled as a quantum channel that introduces error in the quantum states and in some other cases, it is the disorder in the parameters of the Hamiltonian that represent the environmental effects. In yet other cases, it is modelled as a sudden quenching (in time) of the parameters of the Hamiltonian. We have also considered loss of subsystems from among a cluster of systems as a possible form of noise. The results of the dissertations suggest that there is a large class of any-particle quantum states where entanglement and other quantum correlations is sustained even in the resence of environmental effects. These many-particle quantum states can be realized as ground state or excited states of certain many-body systems and hence could be availed for information processing protocols in experiments such as in cold atoms. We connect the result of survival of entanglement in many-particle systems to the fundamental concept of quantum superposition of macroscopic states -- Schroedinger catstates. In cases where quenching in time is considered, we have been able to connect the survival of entanglement to the ergodicity of the corresponding system, a fundamental concept in equilibrium statistical mechanics

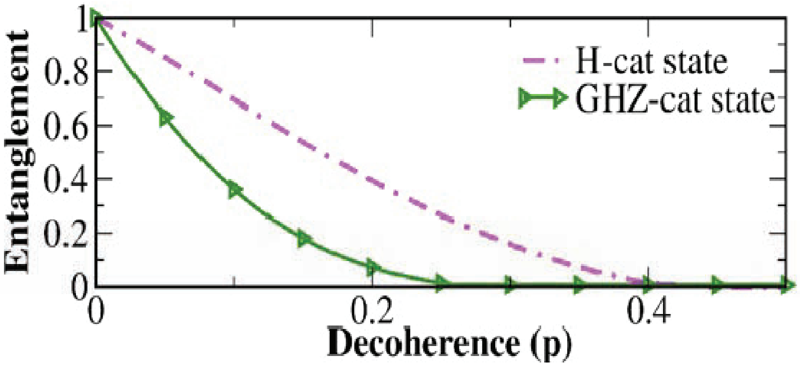


Fig. 1.7.4. Entanglement of the quantum H-cat and GHZ-cat states against local decoherence. The horizontal axis represents a dimensionless (decohering noise) parameter (p), and the vertical axis is the entanglement (in ebits).

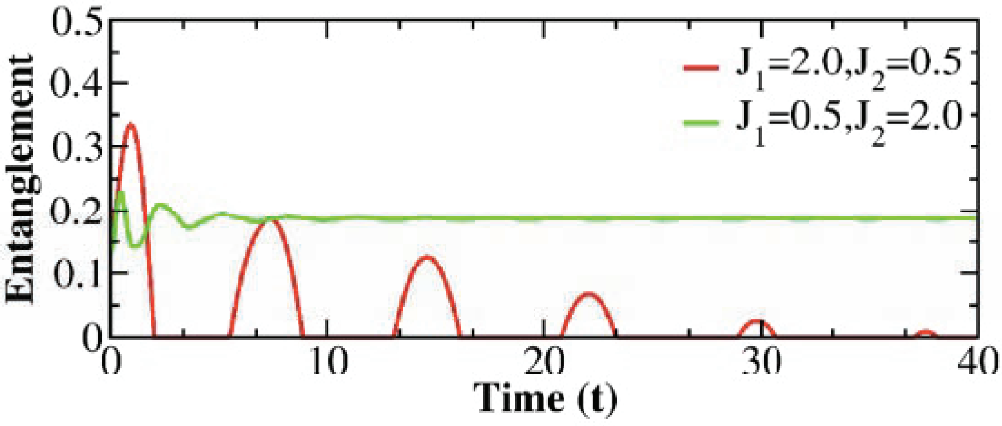


Fig. 1.7.5. Fate of the bipartite entanglement between nearest-neighbor sites against time in a time-dependent quantum XY spin chain when coupling constants are quenched from an initial value (J1) to a final value (J2).

2. Chemical Sciences

During this period, HBNI awarded Ph.D. degree to 40 students who carried out research in the area of Chemical Sciences at different CI/OCC of HBNI. Highlights of research specific to different CI/OCC are as follows.

2.1 Bhabha Atomic Research Centre (BARC), Mumbai

Research related to development of novel sorbents for a variety of contaminants has been pursued. Newpolymeric nano titania-chitosan composite sorbents have been prepared for the removal of cobalt, arsenic and antimony generated during dilute chemical decontaminations of nuclear power plants.The results showed that it is possible to have good control over the properties of the beads prepared through rational choice of composition of the constituents in the pre-polymerisation mixture during preparation of the beads, and by employing suitable solution conditions during sorption. Chitosan tripolyphosphate (CTPP) beads,humic acid coated chitosan trypoliphosphate (HA-CTPP) beadswere used as sorbents for toxic metal ions removal from aqueous solutions. U(VI) was the principal metal ion contaminant, though in certain cases Cr(III) and Pb(II) ions were also used as target pollutants. Metal ion loaded onto CTPP beads were recoverable using simple electrolytes such as NaCl and the adsorbent was found to be effective for Cr(III) removal even in presence of common interfering ions such as Na(I), Ca(II), Mg(II) and Fe(III). In addition, geogenic material impregnated alginate beads, core shell type silica microspheres and humic coated goethite hybrid materials have been studied for their sorption affinity for conventional contaminants like fluoride, arsenic and also radionuclides like U, Pu, Am, Th (Fig. 2.1.1.). The developed materials were tested successfully with contaminated groundwater samples without affecting the water quality parameters. Potable kits were developed for decontamination of groundwater from F, As and U and demonstrated for cleaning of actual ground water samples having F, As and U contamination. On a different note, 1,3-dioctyloxy calix[4]arene-crown-6 (CC-6) and 1,3-dioctyloxy calix[4]arene-benzocrown-6 (CBC) have also been synthesized for the

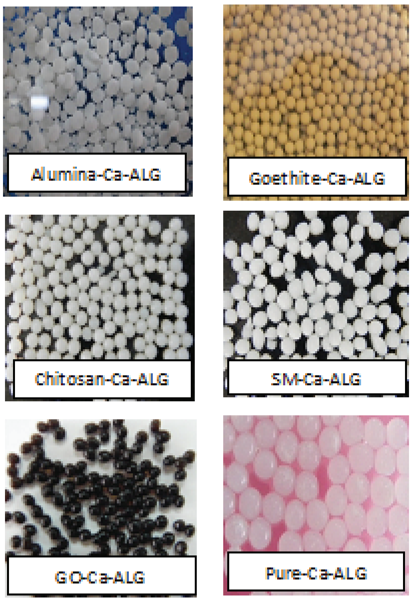


Fig. 2.1.1 Different types of Ca-ALG beads

separation of Cs-137ions from reprocessing waste.Pu(IV)-selective polymer sorbents for the alpha spectrometry and thermal ionization mass spectrometry have been developed.Silica coated superparamagnetic Fe_3O_4 embedded functionalized porous poly(ethersulfone) (PES) beads were developed for the Pu(IV) preconcentration and analysis by TIMS.

Theoretical studies showed that nature has its own mechanism to recognize ions and the selectivity originates either because of structural framework of receptors/binders or because of radionuclide's intrinsic properties. Work has been performed to elucidate the binding and transport mechanism ofradionuclides (Cs^+ and Sr^{2+}) with natural receptors/binders such as soil organic matter (SOM), fulvic acid (FA) and soil microorganisms.Nanofiltration membranes have been developed using sulfonic acid containing diamines like 2,4 – diamino benzene sulfonic acid (DABSA) as well as binary sulfonic acid containing monomers such as 4,4$^{/}$ - diaminostilbene 2,2$^{/}$ - disulfonic acid (DASDSA) and 2,2$^{/}$ - benzene disulfonic acid (BDSA). Several membrane compositions have been investigated using binary and ternary recipes, using these monomers, in combination with other amines like piperazine (PIP) and acid chlorides like trimesoyl chloride (TMC) and terephthaloyl chloride (TPC). Research work was carried out to understand the change in migration behaviour and speciation of uranium in terrestrial environment in response to changes in environmental conditions.The study revealed thatthe extent of migration depends on the speciation of U in the matrix as well as salt types. Salts driven migration process in general follows ion-exchange mechanism whereas, NO_3^- salts mobilize U from solid matrix both by ion exchange as well as oxidative dissolution of U(IV) to U(VI).Geological setup with high ferro-manganese content offers least mobile environment for uranium. Such geological set up offers candidate sites for waste disposal facilities or geological repository of U.

In order to meet the growing demand of rare-earth based materials, better metallurgical technologies are required for the synthesis and engineering scale production of rare-earth metals and their alloys in an efficient and economical way.In this regard, a modified molten salt electrolysis method has been developed to obtain four light rare earth metals i.e. La, Ce, Pr and Nd and some of their alloys i.e. La-Mg and Nd-Fe.Process parameters like temperature of operation, electrolytic composition and cathode current densities have been standardized to get maximum current efficiency and yield in the bulk deposition of metal.A novel polyethersulfone based composite beads encapsulating organic extractant (di-2-ethyl hexyl phosphoric acid (D2EHPA) and 2-ethyl hexyl phosphonic acid (EHEHPA)) have been developed to separate and purify rare-earths (yttrium, dysprosium) from lean and secondary sources. The developmental work also involved evaluation of various additives to alter the beads internal morphology which can maximize the encapsulation and minimize the loss of extractant. Polyvinyl alcohol and multiwall carbon nanotube doped PES/D2EHPA beads (Fig.2.1.2) have shown higher loading capacity (100mg of Dy/gram beads) in comparison to conventional solvent extraction process.A process for rare-earths recovery (Dy from La and Sm) by employing hollow fibre membrane (HFM) contactor module having organophosphorus type of extractant has also been developed.

Fig. 2.1.2: Optical and SEM image of PES/MWCNT/D2EHPA polymeric bead

Considerable research effort has also been directed in the field of hydrogen production, purification and storage. Sulfur-iodine thermochemical cycle is proposed for the large scale production of hydrogen employing nuclear or solar heat.Development of platinum based catalysts with carbon as well as oxides like zirconia, ceria and titaniasupports for hydriodic acid decomposition reaction in liquid phase has been carried out. Zirconia supported catalysts was found to be performing better as compared to the other two oxide catalysts in terms of activity and stability.Pd-based dense metallic membranes for purification of hydrogen isotopes have been developed.$Pd_{0.77}Ag_{0.10}Cu_{0.13}$alloy has been found to be superior to $Pd_{0.77}Ag_{0.23}$alloy for hydrogen purification applications.

Using the density functional theory (DFT) based electronic structure calculations, perovskite based photocatalysts have been designed for the generation of hydrogen via visible light driven water splitting. The various important dopant pairs such as (N,Mo), (N,F), and (Sb, N), (Rh, Sb) were used for $NaTaO_3$ and $SrTiO_3$, respectively (Fig.2.1.3). Another material studied for this purpose was metal decorated porous graphitic carbon nitride ($g\text{-}C_3N_3$).

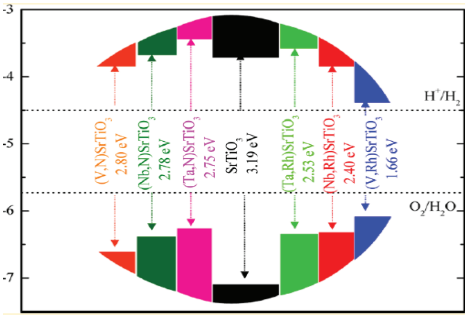


Fig. 2.1.3(a) Enhancement of visible light photocatalytic activity of $SrTiO_3$ by doping

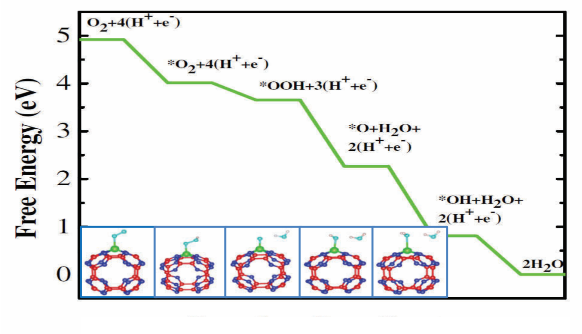


Fig. 2.1.3(b): Metal decorated porphyrin-like porous fullerene as catalyst for oxygen reduction

The hydrogen isotope storage behavior of Zr-Co-M ternary alloys was systematically investigated by generating the hydrogen/deuterium desorption pressure-composition isotherms (PCIs) by employing Sieverts' type apparatus.Alloys of composition $ZrCo_{1-x}Ni_x$(x = 0.1, 0.2 and 0.3), $ZrCo_{0.9}Fe_{0.1}$ and $Zr_{1-x}Ti_xCo$ (x = 0.1, 0.2 and 0.3)were prepared and characterized. Considering the PCT studies, hydrogen induced disproportionation studies and structural studies, it is proposed that among the alloy studied, $Zr_{0.8}Ti_{0.2}Co$ alloy is the best suitable non-pyrophoric and non-radioactive ternary alloy as a substitute for the conventionally used highly pyrophoric uranium bed for tritium storage applications.For the metal hydride to be used as a storage medium, it should satisfy certain requirements such as hydrogen storage capacity, reversibility and wide range of equilibrium plateau of absorption-desorption pressure isotherms and first kinetics. Based on these criteria, uranium, zirconium and their alloys have been considered to be good for storage of tritium.To understand the fundamental properties of these systems, a comprehensive study, both experimental and theoretical, has been carried out. The electronic and thermodynamic properties of $ZrCoX_3$ (X= H, D and T) were carried out using a combined DFT and phonon method.In order to understand the hydrogenation behavior of ZrCo compound, a comprehensive study of hydrogen adsorption on ZrCo surface as well as ZrCo clusters wascarried out. The interaction of hydrogen with the ZrCo cluster indicates the preference of H adsorption on the Co site.Other theoretical studies include study of diffusion behaviour of hydrogen and deuterium in Zr based alloys to understand deuterium ingress in pressure tubes of Pressurised Heavy Water Reactors (PHWRs), development of analytical methodology for determination of total gas in Prototype Fast Breeder Reactor (PFBR) fuel material, studies on the possible use of Pdnanocatalyst for reduction of U(VI) to U(IV) in fuel reprocessing,effect of carbon nanotubes, boron-nitride nanotubes and fullerenes on the molecular properties of water and acid-base complexes and also evaluation of catalytic properties of metal atoms and clusters of titanium, vanadium and gold on a few important reactions such as CO oxidation and water dissociation process.

Atomistic molecular dynamics (MD) simulation, which can provide both structural and dynamical information at atomic scale, has been employed for the exploration of structure and dynamics of water in bulk and at interfaces. Starting from exploring the microscopic details of the local structure of bulk water and its dynamics, thisparticular work proceeds through predicting various properties of heavy water and finally revealing modifications in structure and dynamics of water at molecular as well as nanoscopic interfaces. Exploration of bulk water shows hydrogen bond is the key parameter, which governs structural properties of water. Heavy water is another bulk liquid of immense importance. Structural, dynamical and thermophysical properties of heavy water at a wide range of temperatures have also been estimated by using a newly defined heavy water model

Stress corrosion cracking (SCC) of the structural components fabricated of type 304/304L/304LN stainless steel is the crucial issue for boiling water reactors of (SS). Inhibitive protective coating of zirconia on SS surface is proposed to mitigate the SCC problem. In this context, the mechanism of the growth of zirconia on the SS surface oxide (Fe_2O_3) has been explored. The hydrothermal deposition using $ZrO(NO_3)_2.6H_2O$ salt, Na-EDTA and sodium dodecyl sulphate led to deposition of continuous, tetragonal nano-zirconia coating on pre-oxidized SS surfaces. Corrosion resistance of the ZrO_2 coated samples increased remarkably with the increase in coating thickness and stabilized after the coating thickness of 1 μm which is the optimum thickness for corrosion protection applications.Interaction of aluminide coated Ni-Cr-Fe based superalloy substrates with simulated nuclear waste and borosilicate glass has been studied. The results clearly depicts that low Al containing pack aluminization composition (2 wt.% Al, 2 wt.% NH_4Cl and 96 wt.% Al_2O_3) is acceptable for synthesis of aluminized coatings on Alloy-690 specimens, that is used in metallic and ceramic melter pots for the vitrification of high level nuclear waste.

Ultrafast charge transfer dynamics of quantum dots in absence and in presence of molecular adsorbate has also been explored. The charge transfer dynamics have been demonstrated using CdS QD in presence of 4 ,5 -dibromo fluorescence and two BODIPY (borondipyrromethene derivative) dyes.CdSe/ZnS(Type-I) and CdSe/CdTe(Type-II) core-shell nanoparticles were also synthesized for developing third generation QD solar cell. A new thermoluminescence (TL) materials in $MgAl_2O_4$:C system was also developed.

In the field of synthetic chemistry asymmetric syntheses of some oxygenated heterocyclic compounds have been attempted. To this end, two diverse synthetic strategies were adopted. One of these is based on development of a substrate-controlled asymmetric Barbier-type regioselectivepropargylation and allylation reaction using (*R*)-cyclohexylidene glyceraldehyde as a chiral template. These reactions were also extended to several other aldehydes to expand their scope in organic synthesis. Also coordination/transition metal (Pt/Pd) driven self-assemblies with chalcogen ligands for application as catalysts in C-C coupling reactions have been synthesized.

A series of new surface modification strategies were developed for magnetic nanoparticles for its successful application as drug delivery vehicle, diagnostics and effective heating source for hyperthermia.MNPs conjugated with targeting receptors such as folic acid (FA) and specific luminescent markers like fluorescein isothiocyanate (FITC) can provide detailed understanding of disease-related biological processes at the molecular level (Fig. 2.1.4). In this context, bifunctional magnetic nanoparticles (BMNPs) containing a carboxylic moiety for drug binding and FA for drug targeting were prepared by introducing bioactive cysteine molecules onto the surface of undecenoic acid coated Fe_3O_4 magnetic nanoparticles (UMNPs) via thiol-ene click reaction.

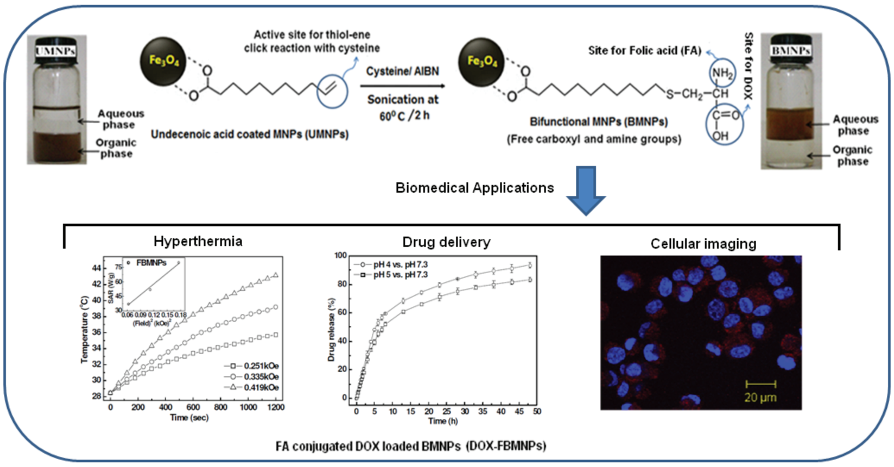


Fig. 2.1.4: Schematic representation of synthesis of folic acid conjugated DOX loaded bifunctional nanoparticles and their biomedical applications

A simple one-pot method for in-situ synthesis of silver nanoparticles (AgNPs), within polyvinyl alcohol-gum acacia (PVA–GA) hydrogel matrix, by γ-radiation induced cross-linking has been explored.Major objective of this study was to determine how the size and rate of leaching out of AgNPs affect the antibacterial activity. It was observed that higher the crosslinking density, smaller is the size of AgNPs and better is the antibacterial activity, even though the rate of leaching is slow. *N*-succinyl chitosan (NSC) based hydrogel beads, stabilized with glycopolymeric network (NSC/Glc-gel), for applications in delivery of anticancer drug doxorubicin (DOX) were developed. The biocompatibility and cell uptake behaviours of Glc-acryl (C-6 acrylamide) and Glc-bis (C-3, C-6 bisacrylamide) were also studied using human intestinal cell lines (INT407), as it contain receptors which can specifically identify D-glucose moieties (Fig. 2.1.5).

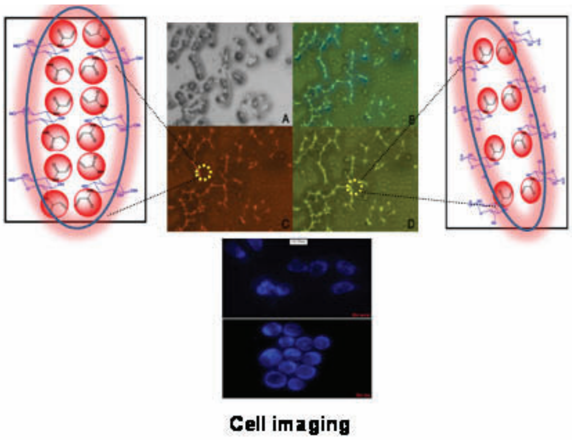


Fig. 2.1.5: Self assembled fluorescent sugars shedding light on lectin recognition and cell imaging

Specific radiotracers have been designed for different tumors making use of different carrier molecules as targeted vectors and also to demonstrate their tumor targeting abilities in diagnostic or therapeutic applications.The use of porphyrins in designing radiolabeled agents for targeting tumor, the mechanisms involvedalong with details of syntheses of different derivatives of porphyrin, their radiolabeling with suitable radionuclides (^{68}Ga, ^{177}Lu and ^{90}Y) and preliminary evaluations in suitable animal tumor models have been studied in detail (Fig. 2.1.6).

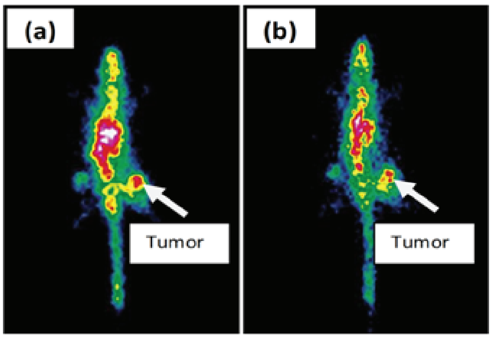


Fig. 2.1.6: Scintigraphic images of tumor bearing Swiss mice exhibiting tumor uptake and retention of ^{177}*Lu labeled porphyrin derivative (a) 16h post injection and (b) 72h post injection.*

2.2 Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam

During the period, 4 students were awarded Ph.D. degree in Chemical Sciences. Highlights from some the theses are presented as follows.

A. Development of a Single-Cycle Approach for Minor Actinide Partitioning

High-level liquid waste (HLLW) is generated during reprocessing of spent nuclear fuels. Partitioning of radiotoxic elements present in HLLW followed by transmutation of them (P&T strategy) into stable or short-lived products in accelerated driven systems or fast-reactors is a viable option for minimizing the radiotoxicity and safe management of HLLW. The current practice of trivalent actinide partitioning is a two cycle approach. It involves the separation of trivalent actinides and lanthanides together from the PUREX raffinate in the first cycle by using neutral extractants such as n-Octyl(phenyl)-N,N-diisobutylCarbamoylMethyl Phosphine Oxide (CMPO), tetra-octyldiglycolamide (TODGA), tetra-2-ethylhexyldiglycolamide (TEHDGA), and tri-octylphosphine oxide etc. followed by lanthanide (Ln)-actinide (An) separation using some acidic extractant such as bis(2-ethylhexyl)diglycolamic acid (HDEHDGA), di-2-ethylhexyl phosphoric acid (HDEHP) etc. in the second-cycle. The product obtained in the first cycle serves as feed solution for the mutual separation of An(III) and Ln(III). Though this involves two- cycle, waste generation, man power is more and not economical. This process may be simplified by combining both neutral and acidic extractant in a single-cycle approach. In single-cycle approach, both trivalent actinides and lanthanides can be extracted from HLLW followed by selective separation of actinides from lanthanides. The present work involves testing of various combinations of neutral and acidic extractant in order to use them in a single-cycle approach and their evaluation for the mutual separation of lanthanides and actinides. Studies reported in the thesis aimed at the development of single-cycle approach for the mutual separation of trivalent actinides from trivalent lanthanides. Several combinations such as unsymmetrical diglycolamide (UDGA) - HDEHDGA, TODGA-HDEHP, TEHDGA - HDEHP etc. are studied to examine the feasibility of mutual separation of trivalent lanthanides and actinides.

B. Studies related to spent fuel reprocessing using tri-iso-amyl phosphate as an alternate extractant to tri-n-butyl phosphate

High-level liquid waste (HLLW) is generated during reprocessing of spent nuclear fuels. Partitioning of radiotoxic elements present in HLLW followed by transmutation of them (P&T strategy) into stable or short-lived products in accelerated driven systems or fast-reactors is a viable option for minimizing the radiotoxicity and safe management of HLLW. The current practice of trivalent actinide partitioning is a two cycle approach. It involves the separation of trivalent actinides and lanthanides together from the PUREX raffinate in the first cycle by using neutral extractants such as CMPO, TODGA, N,N,N',N'-tetra-2-ethylhexyldiglycolamide (TEHDGA), and tri-octylphosphine oxide (TOPO) etc, followed by lanthanide (Ln)-actinide (An) separation. The product obtained in the first cycle serves as feed solution for the mutual separation of An(III) and Ln(III). The nitric acid concentration of the above aqueous product varies from 0.1 M to 0.001 M. The present work involves the synthesis of various diglycolamic acid based extractants and their evaluation for the mutual separation of lanthanides and actinides. Studies reported in the thesis aimed at the development of diglycolamic acid class of extractants having desirable properties for the mutual separation of trivalent actinides from trivalent lanthanides and vice-versa. Several alkyldiglycolamic acids have been synthesized and studied to examine the feasibility of using them for the mutual separation of trivalent lanthanides and actinides by liquid-liquid extraction as well as solid-liquid extraction route.

Two extractants bis(2-ethylhexyl)diglycolamic acid (HDEHDGA) and its sulfur derivative, bis(2-ethylhexyl)thiodiglycolamic acid (HDEHSDGA) were developed for the mutual separation of lanthanides and actinides by liquid-liquid extraction method. HDEHSDGA shows the potential of separating actinides from lanthanides in a single contact with a separation factor of ~2600 at pH 3. A method was also developed for the demonstration of mutual separation of Am(III) and Eu(III) from dilute nitric acid medium by using a solution of 0.1 M HDEHDGA/n-DD. Unlike the other lanthanide-actinide separating extractants in use, HDEHDGA was made up of CHON- atoms and compatible with a nuclear diluent, n-dodecane. Solid phase extraction is a promising technique for the separation of metal ions from aqueous solution owing to its simplicity, robustness, regenerating ability and can be easily engineered into plant scale levels and technologically demonstrated. In fact, solid phase extraction is suitable for the separation of micro-quantities of radionuclides present in a large volume of feed solution, as in the present case. In connection with these, several of solid phase adsorbents were developed and studied the feasibility of using them for the mutual separation of lanthanides and actinides. A number of solvent impregnated resins were prepared by impregnating the alkyl derivatives of diglycolamic acid with alkyl group varied from butyl to decyl group, for the mutual separation of Am(III) and Eu(III), by extraction chromatography. Among the diglycolamic acids prepared, octyl diglycolamic acid impregnated resin showed the superior potential for the mutual separation of Eu(III) and Am(III) by extraction chromatography. Another adsorbent was prepared by polyamine resin matrix, chemically modified with diglycoamic acid, diglycolamic acid (PA-DGAH), and studied for the extraction of americium(III) and europium(III) from dilute nitric acid medium. The results of the extraction studes confirmed the feasibility of separating Am(III) from Eu(III) with a separation factor of ~45 by using PA-DGAH. These chemically modified resins have superior chemical stability as compared to impregnated resins. To overcome the problems associated with radiolytic degradation and disposal of spent organic resins, chemically inert inorganic solid supports such as silica grafted with various organic compounds have been studied for the efficient removal of metal ions from waste streams. A diglycolamic acid functionalized silica gel (Si-DGAH) was prepared and studied for the separation of americium(III) and europium(III) from dilute nitric acid medium and the results of the study confirmed the possibility of using Si-DGAH for the mutual separation lanthanides and actinides from dilute nitric acid medium. Magntic Solid Phase Separation (MSPS) is another promising technique for the separation of toxic and radiotoxic metal ions from various aqueous streams. In the MSPS technique, the magnetic particles (MPs) are added to the waste solution to extract the target metal ion. The MPs are then separated from the solution by means of an external magnetic force. A couple of magnetic solid phase adsorbents Fe-DGAH and Fe-SDGAH were also synthesized and studied for separating trivalent lanthanides and actinides. The extraction studies with these adsorbents confirmed the feasibility of separating Am(III) from Eu(III) with a separation factor of ~150 by using Fe-DGAH

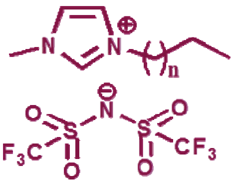
C. Development of extractants for the mutual separation of lanthanides and actinides
Tri-n-butyl phosphate (TBP) in dodecane has been employed as a solvent for various separation processes in nuclear industry. However, the experience gained in the last six decades has brought out a few drawbacks of TBP that are of concern during reprocessing of spent fast reactor fuels. The major drawbacks of TBP include third phase formation with tetravalent metal ions e.g. Pu(IV), higher aqueous solubility, radiation degradation etc. Several symmetrical trialkyl phosphates (TalP) have been investigated in our laboratory towards identification of an alternate extractant to TBP for fast reactor fuel reprocessing and these studies have indicated tri-iso-amyl phosphate (TiAP) as a suitable extractant.

Prior to the deployment of a novel solvent, TiAP /n-dodecane (n-DD) in an actual reprocessing plant, it is essential to understand the various aspects of this solvent system. In this context, the present study mainly focused on the issues arising from reprocessing of fast reactor fuels. The extraction behavior of actinides (U, Pu and Am), troublesome fission products (e.g. Zr, Ru, Tc) and some of the lanthanides (La, Pr, Nd, Sm, Eu) as fission product representatives with TiAP were investigated and compared with the TBP/n-DD system under identical experimental conditions. Continuous counter-current solvent extraction runs with TiAP based solvent using a mixer-settler have been carried out under various experimental conditions. Preliminary studies have been also carried out to develop an alternate method for the processing of metallic alloy fuels by aqueous route using PUREX process with TiAP based system. Thermal and radiolytic stability of TiAP system have been investigated and the results of TiAP solvent are compared with TBP. Studies carried out in the present work on various physicochemical and extraction properties as well as third phase formation phenomena have established that tri-iso-amyl phosphate is a suitable extractant for fast reactor fuel reprocessing.

2.3 National Institute for Science Education and Research (NISER), Bhubaneswar

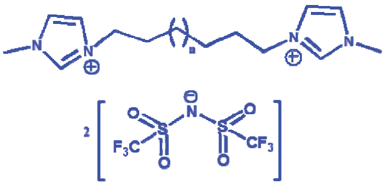
During the period, 9 students were awarded Ph.D. degree in Chemical Sciences. Highlights from some the theses are presented as follows.

One thesis is focused to understand the kinship among structure, intermolecular interactions and dynamics through solute and solvent dynamics study in mono and dicationic room-temperature ionic liquids (RTILs) by employing steady-state and time-resolved fluorescence as well as Nuclear Magnetic Resonance (NMR) studies. Outcome of the present thesis are summarised as follows. (1) Electrostatic (ion-ion) interaction is observed to significantly hinder the rotational relaxation of charged solutes. (2) It has been observed that the rate of solvation dynamics can influence the rate of intramolecularphotoinduced electron transfer (PET) process in a significant manner. (3) Nature of intermolecular interaction for different IL-cosolvent systems has been observed to be different. (4) It has been demonstrated that the chain length of alkyl group (terminal/bridge) plays important role in determining nanostructural organization in monocationic ILs (MILs) and dicationic ILs (DILs) (Figure 1). (5) Dipolar rotation of the imidazoliumcation is found to be responsible for ultrafast component of solvation that are usually observed in imidazolium-based ILs. (5) The dynamical behaviour of the DILs are observed to be quite different from that of usual MILs.



1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide

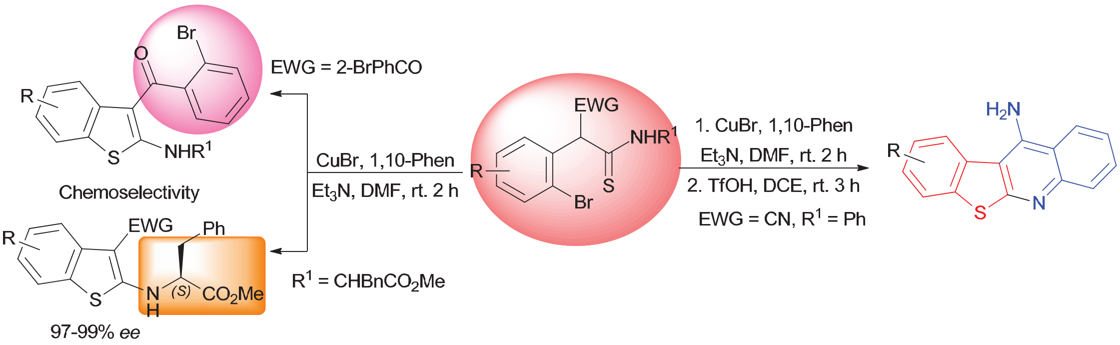
n= 1, $[C_3MIm][NTf_2]$
n= 4, $[C_6MIm][NTf_2]$



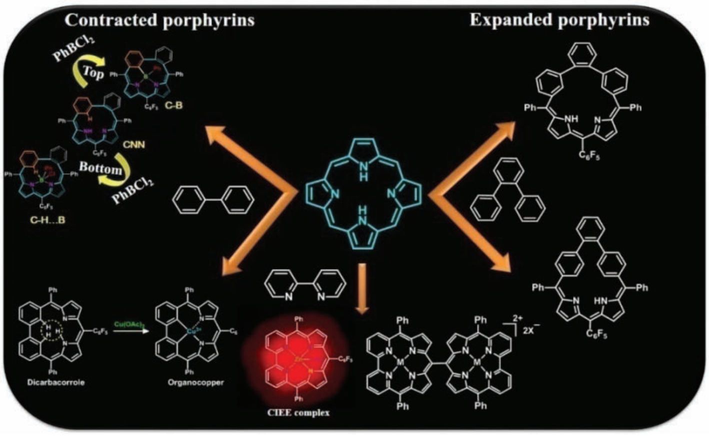
1,6-bis-(3-methylimidazolium-1-yl)hexane bis(trifluoromethylsulfonyl)amide

n= 1, $[C_6(MIm)_2][NTf_2]_2$

The first general and efficient method for trideuteromethoxylation of aryl/heteroaryl halides with CD_3OD using a commercial available ^{t}BuXPhos ligand and $Pd(OAc)_2$ was developed. This was further extended to selective catalytic deuteration of halo arene/heteroarenes. A mild and practical method for the synthesis 2-aminobenzo[b]thiophenes, which involves a copper-catalyzed chemoselectiveintramolecular Ullman reaction of thioamides at room temperature for the first time was achieved (Scheme 1). This observation was opened-up a novel synthetic protocol for designing various heterocyclic compounds at room temperature.

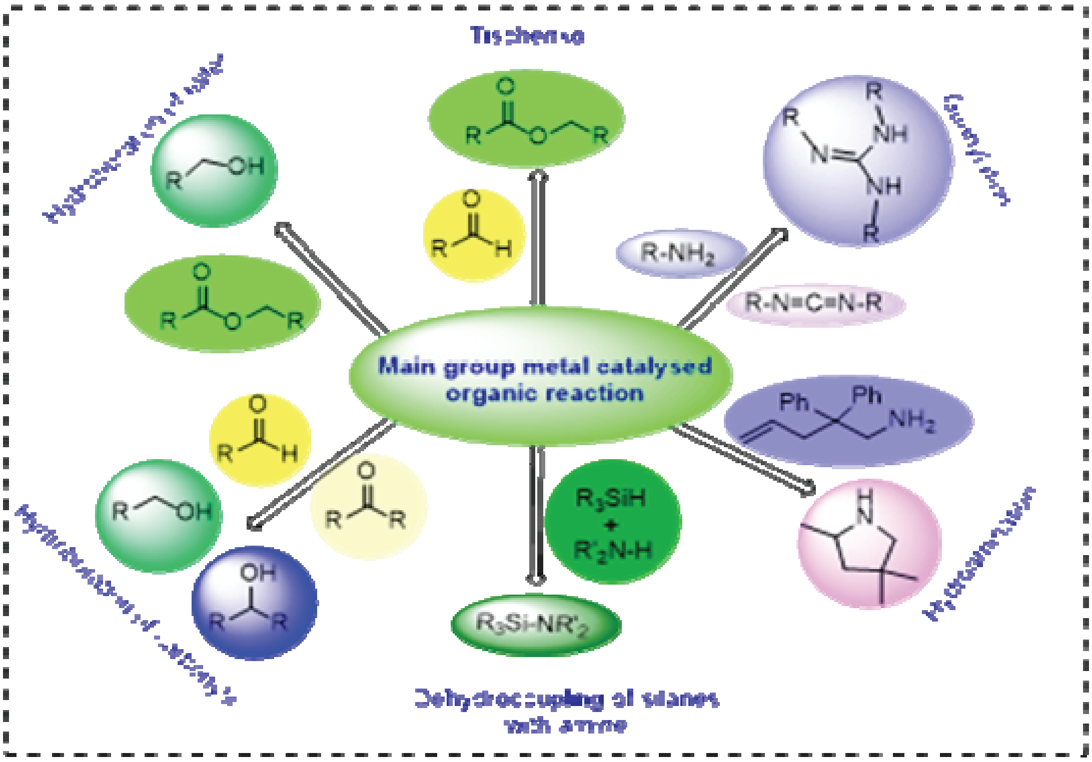


In this thesis work, it is successfully embedded the bipyridine, biphenyl and terphenyl systems into the porphyrin framework. These molecules are further explored for the following properties; (i) Biphenylcorrole with adj-CCNN core is effectively utilized for stabilizing organocopper(III) complex; (ii) the monoanionicBipyricorrole binds with Zn^{II} ion and further exploited the metal ion sensing experiments for the selective detection of Zn^{II} ion; (iii) the smallest contracted porphyrin analogue Carbatriphyrin(3.1.1) – is found sutable to stabilize organoborane and also demonstrated the weak C-H…B interactions; (iv) similarly, the smallest expanded porphyrinoid, carba-homoporphyrins(2.1.1.1) coordinates with Rh(I) ion in the macrocyclic framework; v) finally, serendipitously discovered the metal template synthesis of meso-free bipyricorrole in the absence of any acid-catalysts as well as oxidizing agents and further utilized it for the oxidative coupling reactions. Overall, the synthesis of novel homologues and analogues of contracted and expanded porphyrinoids by introducing the polycyclic aromatic units in the macrocyclic framework are provide ideal platform to explore diverse applications. Also highlights the reactivity, receptor property and coordination chemistry of these macrocycles. These macrocycles pave the way for the various metalion insertion, aromatic properties, catalysis and sensing studies.



A wide range of main group metal complexes bearing bulky guanidinate ligands have been synthesized and structurally characterized. Moreover, these metal complexes have been utilized as (pre)-catalysts for various organic transformations.

This thesis deals with the synthesis and characterization of magnesium and zinc complexes bearing neutral N-heterocyclic carbenes and “NHC-CDI” adducts or zwitterionicamidinate ligands. Furthermore, NHC supported magnesium complexes have been utilized as pre-catalysts for cross dehydrocoupling and C-N bond formation in guanylation of amines to carbodiimides reactions.



3. Engineering Sciences

During this period, HBNI awarded Ph.D. degree to 46 students who carried out research in the area of Engineering Sciences at different Constituent Institutes (CI) of HBNI. Highlights of research specific to different CIs are as follows.

3.1 Bhabha Atomic Research Centre (BARC), Mumbai

A wide spectrum of research work, encompassing various programmes of the department of atomic energy (DAE), was undertaken in BARC under the Ph.D. programme in engineering sciences. These studies resulted in many interesting and beneficial outcomes. The results have been published in various reputed international peer reviewed journals with high impact. Twenty students received Ph.D. degrees during the period.

A brief report on some of the salient academic and technological outcomes of these studies is presented below.

One thesis focused on the analysis of the issues related to the design and optimization of an efficient Flywheel Energy Storage System. Studies have been carried out to identify the sources of various losses and techniques for reducing them. Factors which influence the quantity of energy harvested have been identified. A patented novel scheme has been proposed which uses a unique combination of multi- armature winding permanent magnet brushless dc machine and a buck converter to maintain the dc bus voltage. Physical design, prototype fabrication of various topologies of energy harvesting system has been carried out. Effect of generator parameters on the on harvestable energy and controller performance is analyzed which confirms 15 – 20% enhancement in the harvested energy from the flywheel, in comparison with other schemes.

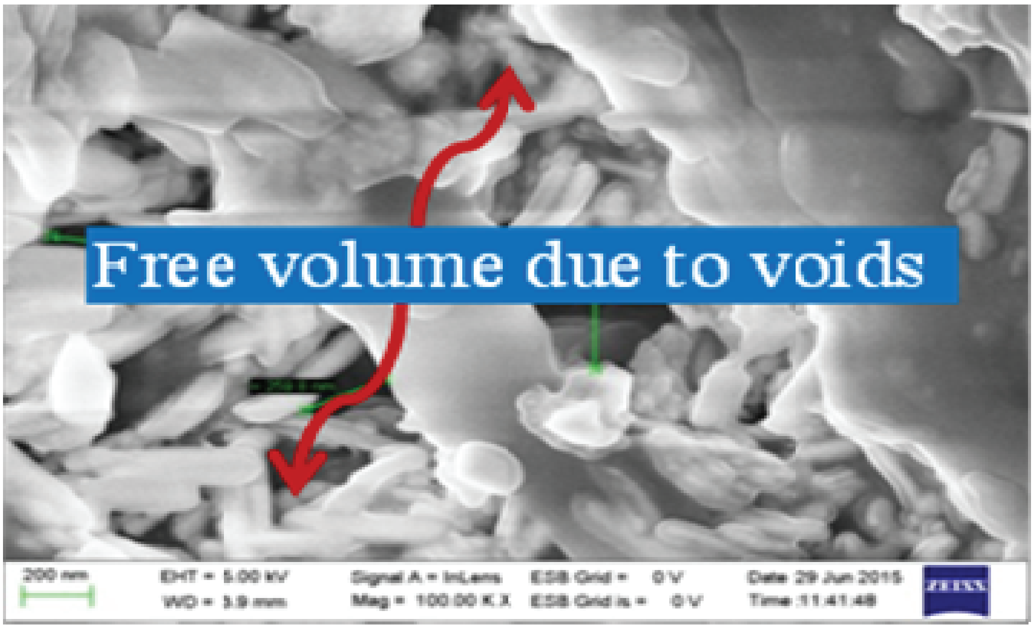


Figure 3.1.1. Experimental facility for PM-BLDC machine based Flywheel Energy Storage System

The thesis of another student titled “Development of Remaining Life Prediction Models for Instrumentation and Control (I&C) Cables for use in Reliability Assessment of NPP Systems “, studies the thermal and radiation ageing of polymeric Instrumentation and control (I&C) cables used for safety-related equipment in Nuclear Power Plants. Experimental methods (e.g. scanning electron microscopy (SEM)) were used to study the degradation mechanisms e.g., formation of voids, and degradation of electrical and mechanical properties (e.g. Insulation Resistance and Elongation-at-Break). Theoretical models using Artificial Neural Network (ANN) were used to determine the time-dependent reliability of the cable and its impact on the safety of the plant.

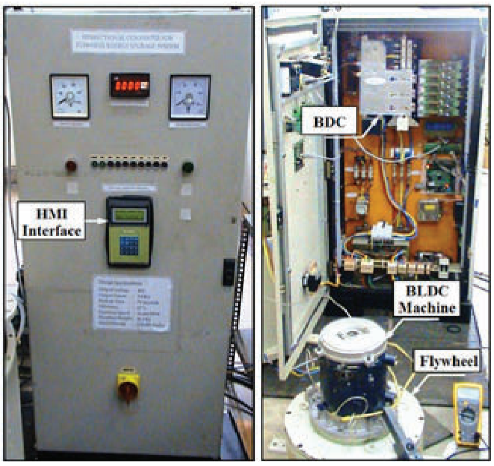


Fig. 3.1.2. SEM Study on Cable Insulation Degradation

The thesis titled “Computation of Neutron Flux Distribution in Large Nuclear Reactors Via Reduced Order Modeling” addressed the problem of monitoring and control of time-varying axial and radial flux distribution in operational large reactors such as Advanced Heavy Water Reactor (AHWR).It focused on the design of a flux mapping algorithm which accounts the time variation of neutron flux distribution as well as random noise in detector readings. The concept of application of Kalman filtering theory has been extended to the near optimal estimation of core flux distribution in AHWR. Different approaches of obtaining reduced order model from the original higher order estimation model of AHWR viz., Davison's, Marshall's, singular perturbation and balanced truncation techniques have been explored to solve the numerical ill-conditioning in Kalman filter design. The study also resulted in a novel technique based on two-time-scale formulation of Kalman filtering problem for the time-dependent neutron diffusion equation to near-optimum estimation of the core flux profile in the AHWR. The important aspect of this technique is that it attempts solving for smaller order state prediction equations, process covariance matrices and Kalman gain.

The thesis entitled “Analytical Design and Development of Resonant Converter Based Fast Capacitor

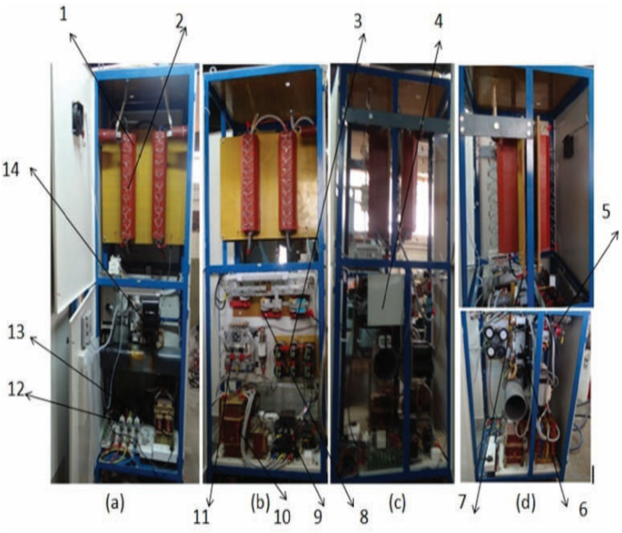


Figure 3.1.2. Experimental Facility for Conducted Noise Analysis and protection of 45 kJ/s, ±50 kV Capacitor Charging Power Supply when Interfaced with Repetitive Marx Based Pulse Power Syste

Charging Power Supply (>40 kJ/s)“ reports work on a topic of practical interest. The thesis reports on repetitive fast capacitor charging power supply (CCPS) that makes use of resonant power conversion stage. Fourth order resonant networks are considered. Various topologies have been attempted with focus on different aspects of a CCPS. The importance of this research is that, high power microwave and charge-particle beam applications have, as usually, very unstable, dynamically –changed in time and repetitive –rate load that effect the process of the pulsed power source operation as well as its charging/discharging dynamics. Detailed analysis, design, fabrication and experiments have been presented.

The thesis on “Study of Beam Dynamics in 100 MeV, 100 kW RF Electron Beam” has focused on the beam dynamics of linear accelerator by analytical methods and computer simulations in order to predict the behavior and quality of the electron beam and minimize the beam loss. In this work, study has been made of the beam dynamics of a 30 MeV standing wave, biperiodic, coupled cavity RF electron Linac with the help of CST Microwave studio and ASTRA code to determine the optimized parameters for a nominal gain of energy of 30 MeV with minimum energy spread and keep the minimal growth of transverse emittance. This facilitates a safety operation of the Linac and avoids induced radioactivity with hands on maintenance of the accelerating structure and components. Two important phenomena: effect of spherical aberrations in axial -symmetric focusing lens and influence of nonlinear space charge forces on beam emittance growth are discussed for different beam distributions. Chromatic aberration induced growth of emittance and distortion of phase space area are discussed. A new formulation for the aperture coupling problem in terms of Carlson Symmetric Integrals has been attempted. The significance of such a method is that it considers the thickness of the aperture in to account to find the coupling coefficients between cavities unlike the earlier works which neglect the thickness of the aperture in aperture coupling problems.

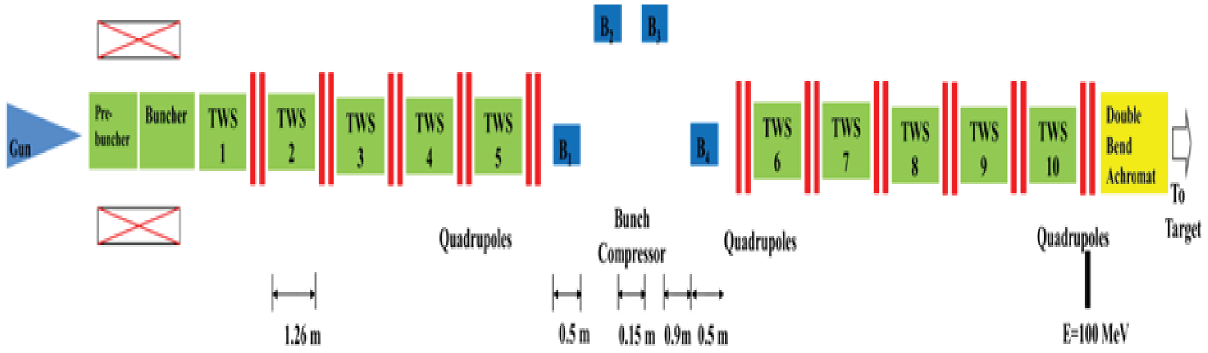
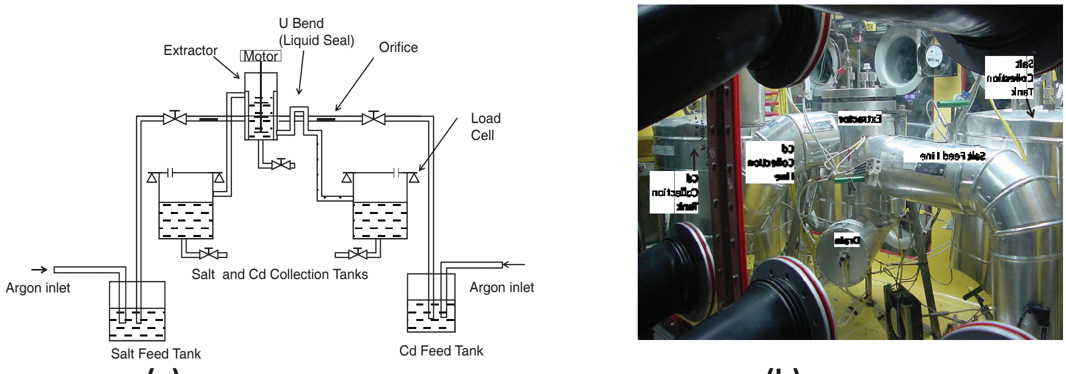


Fig. 3.1.4. Schematic of 100 MeV Travelling Wave Linac

3.2 Indira Gandhi Centre for Atomic Research (IGCAR), Kalpakkam

During the period, 20 students were awarded Ph.D. degree in Engineering Sciences. Highlights from some the theses are presented as follows.One thesis deals with the pyrochemical reprocessing of metallic fuels by molten salt electrorefining. Actinide draw down process is the key step in the molten salt electrorefining used to reduce the waste volume by treating and recycling the electrolyte. The high temperature process carried out at 500° C involves the reductive extraction of actinides from a molten LiCl-KCl salt mixture using Li-Cd alloy as the solvent. In the solvent extraction process, creation of large interfacial area is essential for mass transfer between the phases. In molten salt extraction, the density difference between the phases (6400 kg/m^3) and the interfacial tension (450 dyne/cm) are high which requires more energy to disperse one phase in to other phase. The influence of high density difference on dispersion is studied by conducting experiments on solid –liquid dispersion in a stirred glass vessel using rotating impeller. The low density floating particles with the size range from 100 to 325 micron and room temperature liquid medium with different density and viscosity were employed in this study. A correlation was developed using standard dimensionless group to predict the minimum impeller speed requiredtwo phase dispersion.A laboratory scale molten salt extraction setup with 500 ml continuous agitated extractor was developed for conducting molten salt experiments at 500° C. This set up is installed in aninertatmosphere glove box with argon gas purification system. The flow rate of both salt and cadmium alloy phases were maintained at 25 ml/min by using the orifice in the feed lines. The natural uranium is taken as the solute in the feed salt at a concentration of 0.5 wt %. The percentage extraction of uranium was observed more than 95 % in the extraction experiments.



(a) **(b)**

Fig. 3.2.1.(a) Process flow diagram of the Actinide draw down process (b) Photograph of the high temperature molten salt extraction setup with heaters

The fuel discharged from a nuclear reactor after irradiation still contains most of the fertile material (U^{238} or Th^{232}) which was also the major constituent of the virgin fuel, significant amounts valuable fissile nuclides

(U^{235}, U^{239} and/or U^{233}) and large amounts of fission products. Reprocessing of the spent fuel is aimed at (1) recovering uranium and plutonium and thorium if present, for reuse as nuclear fuels and (2) removing the fission products. Pyrochemical reprocessing is one of the non-aqueous processes and among them; molten salt electrorefining is a pyrochemical reprocessing method especially advantageous for treating metallic fuels from FBR's.

The following modeling and experimental work on the design of electrodes for the electrorefiner were carried out in this study and these will be discussed in the thesis: Developed the model for the electrorefining process using COMSOL Multiphysics in which three modules of the software were coupled together and studied the electrotransport behavior of uranium and plutonium from liquid cadmium anode to solid cathode and validated the model with experimental data from literature.

Developed the model to study the effect of the electrode configuration for achieving higher throughput and validated the model with experimental studies carried out by us as well as with experimental data from literature. Also studied the electrodeposition of uranium using different shapes of the cathode both by modeling and by experimental work.

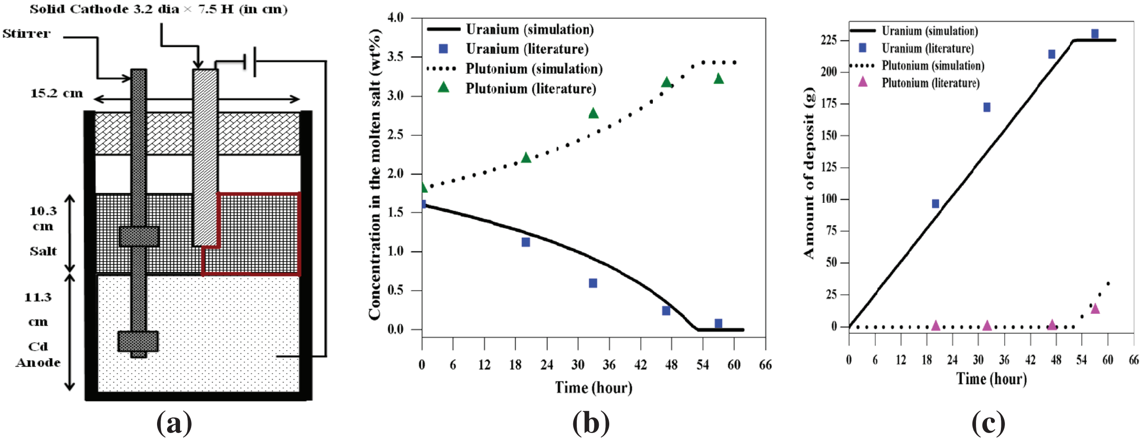


Fig. 3.2.2. (a) ANL laboratory scale Electrorefiner. Colored portion is used for 2D axis-symmetrical model, (b) Concentration of uranium and plutonium in the molten salt - model validation with experimental data from literature, (c) Deposition histories of uranium and plutonium on the solid cathode - model validation with experimental data.

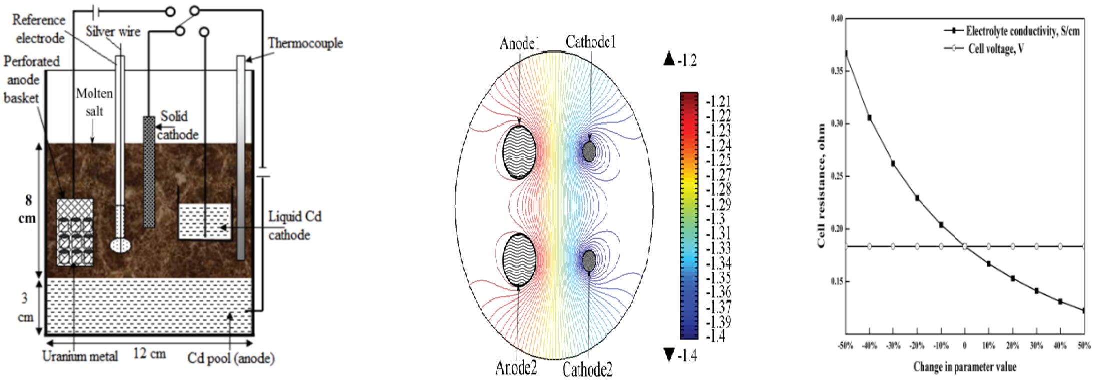
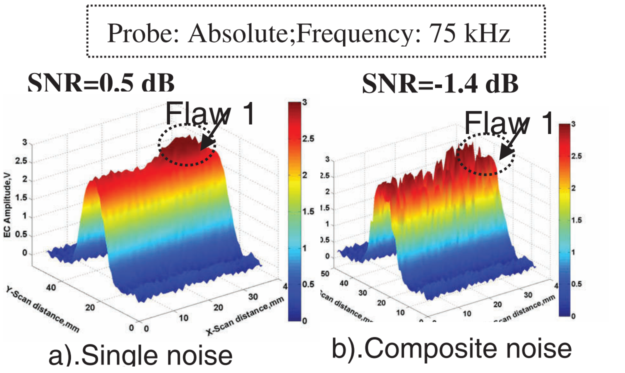


Fig. 3.2.3. (a) Schematic of the experimental electrorefiner is operated with 3 separate arrangements (a) Cd pool anode – solid cathode (b) Cd pool anode -liquid Cd cathode (c) Perforated anode basket – solid cathode, (b) Potential distributions for the parallel arrangement of electrodes, (c) The effect of changes in parameters on Cell resistance

Simulated the concentration variation of U and Pu and Pu/U ratio's in the molten salt, liquid cadmium anode and amount of U deposit on the solid cathode and validated with literature data. Also predicted the cell voltage and compared with literature data. Evaluated the potential and current density distributions, measured the current and calculated the cell resistance. Compared the cell resistance of present model with present experimental results and also with literature. Electrodepositions of uranium on three different shapes of cathode were performed. As a first approach, taken equal surface areas and in the second approach maintained equal immersion height. The validated results of present model are good agreement with the experimental results.

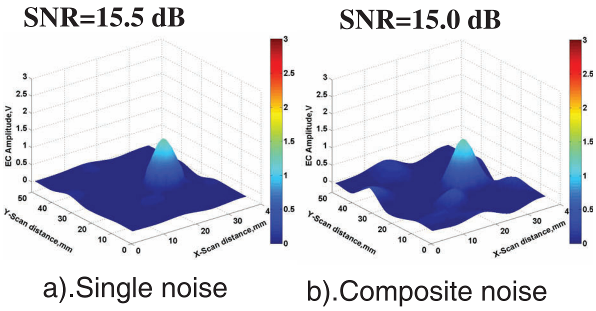
Eddy current nondestructive (EC NDE) technique plays an important role in ensuring structural integrity of thin electrically conducting materials through detection and sizing of flaws. However, it is simultaneously influenced by several variables such as surface roughness, variations in probe lift-off, variations in electrical conductivity and magnetic permeability and variations in geometry, apart from flaws. Fig. 3.2.4(a) shows EC image from a weld region having a surface flaw (Flaw 1) of depth 0.5 mm at constant lift-off (0.3 mm), and noise due to material property variations resulting a Signal to noise ratio (SNR) of 0.5 dB. Fig.1b shows the EC image from the same weld region obtained by varying lift-off 0.0 mm to 1.0 mm, degrades the SNR to -1.4 dB and reduces the sensitivity to detect shallow flaw. The presence of such composite noise is challenging and time consuming, as it involves the use of several methods of processing depending on the source of noise. In view of this, this thesis has laid foundation for automated removal of noise in eddy current images by identifying frequency dependency of flaws and statistical independency of noise and has established three approaches, a)incorporating automated selection of optimum filter and decomposition level in Discrete Wavelet Transform (DWT), b)by establishing an iterative estimation of de-mixing matrix in Independent Component Analysis (ICA) and c)combining the advantages of the flaw retention ability of ICA based approach and the noise reduction ability of DWT based approach (hybrid ICA-DWT based approach) for reduction composite noise in eddy current images.

A significant improvement in SNR of 15.0 dB has been achieved and is shown in Figs. 3.3.5(a) and (b). The proposed hybrid ICA-DWT based approach has not influenced by varying test frequencies (20 kHz-150 kHz) and varying diameter of probe(3.0- 20.0 mm) and has established its noise tolerance up to the variations in lift-off of 0.0 mm to 1.5 mm and could detect shallow flaws (depth<10% wall thickness) of comparable amplitude with that of noise and enables early detection of flaws in components to prevent catastrophic failures.



a).Single noise b).Composite noise

Fig.3.2.4. EC images of a flaw (1) (length 6.0 mm, width 0.25 mm) with (a) material properties variations and (b) composite noise.



a).Single noise b).Composite noise

Figs.3.2.5(a) and (b) Performance evaluation of the hybrid ICA-DWT for variations in composite noise.

Engineering components such as storage tanks are made by austenitic stainless steels with thickness in the range of 8.0 mm to 12.0 mm. These components undergo uniform corrosion, localized pitting and stress corrosion cracking on the inner surface. Inspection of these components surface for corrosion is essential to ensure the structural integrity. The conventional eddy current testing technique is confined to detection of sub-surface flaws within a depth of 5.0 mm in austenitic stainless steel components due to the skin-effect phenomenon. Due to the radiation environment, detection of inside flaws (deep sub-surface) from outer surface is a challenging application of eddy current testing. Further, rapid automated flaw detection is essential for ensuring high probability of detection as well as minimal dose of radiation for the inspection personnel. Hence, for reliable detection and rapid imaging of sub-surface flaws in austenitic stainless steel components, this thesis has proposed novel methodologies.

Research work focused on design and development of high throughput probes which enable higher strength of the primary magnetic field for deeper penetration of eddy currents into the steel. Finite element modelling based comparative studies were carried out using COMSOL multi-physics software for optimization of probe configuration of send-receive type cup-core probe and its dimensions. A high-sensitive eddy current instrument that can drive higher current and implement lock-in amplifier based I/Q technique has been designed and developed for reliable detection of deep sub-surface flaws. The excitation unit in the instrument was specially designed to drive a higher excitation current upto 1A into the probe coil and digital lock-in amplifier was designed and implemented using LabVIEW software for precise measurement of phase lag of the sinusoid from flaws. Surface and sub-surface flaws could be distinguished from the change in phase angle sign. To further enhance the detectability of sub-surface flaws with higher signal to noise ratio (SNR), research work proposed a novel BayWT based image fusion methodology that combined wavelet transform and Bayesian methodologies. Performance of this fusion methodology was compared with that Laplacian pyramid, wavelet transform, principal component and Bayesian based image fusion methodologies. The proposed BayWT fusion methodology has enhanced the flaw detection sensitivity and has resulted in 3 times improvement in SNR. Research work proposed a novel scan plan for rapid detection and imaging of sub-surface flaws which is essential for radioactive environment, after performing detailed systematic studies using raster, diagonal raster, spiral, Lissajous and billiard scan plans.

These developed methodologies were successfully applied to 12.0 mm thick AISI type 304L stainless steel plates for detection of flat bottom holes (simulating sub-surface localized corrosion) and EDM notches (simulating sub-surface cracks). The methodologies presented in this thesis demonstrated the synergistic combination of cup-core coil probe and high sensitive eddy current instrument ensures reliable detection of flaws located 8.0 mm below the surface and also imaging of flaws using the novel BayWT based image fusion methodology. This study has established, for the first time, that the billiard scan plan is an attractive scan plan for rapid and reliable eddy current imaging of flaws in large surfaces of electrically conducting materials.

Mechanical properties of multiphase structural alloys are governed by their microstructural constituents (individual phases/precipitates). With the knowledge of the properties of the individual phases/precipitates, one can study and understand, the stress distribution at micro-scale, the deformation behavior, the crack nucleation, dislocation activity and interaction with grain boundaries and the crack propagation. Thus, the understanding of the response of multiphase materials against external load/strain can be enhanced, which in-turn plays a major role in development of materials with property enhancement and mechanistic understanding.

Atomic force acoustic microscopy (AFAM) was used for mapping the elastic modulus of various phases/precipitates present in two main classes of multiphase structural alloys viz. nickel and titanium alloys, at nanoscale. The microstructure of the multiphase alloys were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), electron back scatter diffraction (EBSD) and Atomic force microscopy (AFM) studies. Specific software were developed to acquire and analyze the data obtained by AFAM system.

In nickel base superalloys, a polycrystalline superalloy, alloy 625 and a directionally solidified superalloy, CM 247A were taken for study. A new methodology was developed to circumvent the problem of change in tip radius by implementing simultaneous acquisition of two contact resonance frequencies and by using matrix as a reference. Cantilever dynamics model neglecting damping was used to derive the contact stiffness (k*) and indentation modulus (M). Experimental M values of γ′, δ and carbides present in the two nickel base superalloys were reported for the first time.

Simultaneous mapping of stiffness and damping was carried out in two types of titanium base alloys viz. Ti-6Al-4V, an α+β titanium alloy (refer below figure) and Ti-10V-4.5Fe-1.5Al, a β titanium alloy [4]. Specimens of titanium alloys were subjected to heat treatment at different temperatures. Cantilever dynamics model considering damping was used to derive the M and damping (*E″/E′*). The experimental *M* and *E″/E′* values of *α*, *β* and *α′* phases present in the two titanium alloys were reported for the first time. Effect of heat treatment on the elastic and damping properties was studied. The elastic and damping properties at nanoscale are compared with those for bulk samples obtained by ultrasonic measurements. The study demonstrated that the nanoscale elastic properties measured using AFAM can also be used for obtaining the average elastic properties of the bulk samples with an accuracy of ~5 %.[4] The systematic error in the elastic property measurements using single reference has also been brought out.

Attempts were made to understand the effect of crystallographic orientation on AFAM measurements. It was demonstrated that, due to the close packed orientation relationships of precipitates with the matrix, the modulus of a precipitate measured by the methodology described in the present thesis was not affected to a large extent by the orientation of individual grain in which the measurement was made. The study also clearly demonstrates that, AFAM can be used to disclose relative elastic property of materials with high spatial resolutions, even for materials with a slight difference in elastic properties (~4 %).

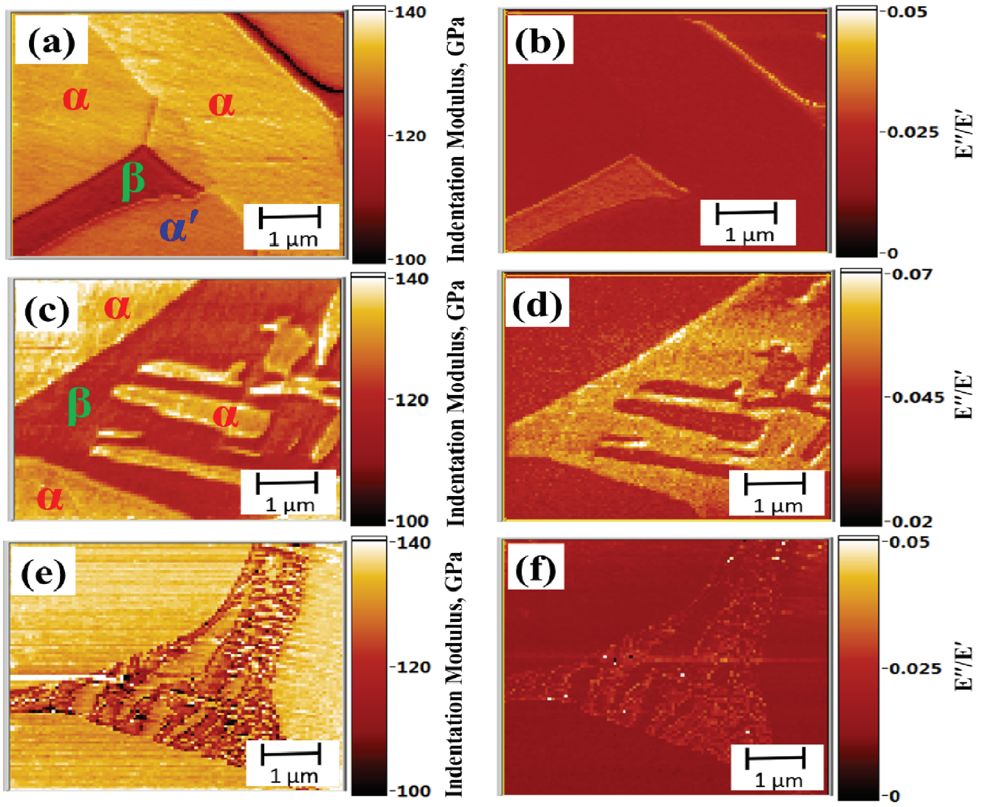


Fig. 3.2.6. Modulus and damping maps of the Ti-6Al-4V specimens heat treated at (a and b) 1223 K, (c and d) 1123 K, and (e and f) 923 K for 1 hour, followed bywater quenching, respectively.

This thesis is focused towards, (i) common cause failure analysis for engineered safety systems using alpha factors obtained by mapping technique, (ii) dynamic modelling of the scenarios with time dependent success criteria and (iii) development of an integrated approach to assess the risk from multi unit nuclear power plants sites with consideration of both external and internal hazards.

In the first part of the research work, common cause failure analysis for engineered safety systems using alpha factors obtained by mapping technique is carried out. Here an approach described in NUREG/CR-5500 is extended in this study to derive plant specific coefficients for CCF analysis especially for high redundant systems. A critical comparison of alpha factor method and beta factor method is also performed by taking insights from the case studies of engineered safety systems installed in existent nuclear power plants.

In the second part of the research work "Markov Analysis for Time Dependent Success Criteria of Passive Decay Heat Removal System" is carried out. The approach described can be used to dynamically model the scenarios with time dependent success criteria in a comprehensive manner and to study various factors affecting the availability of such systems.

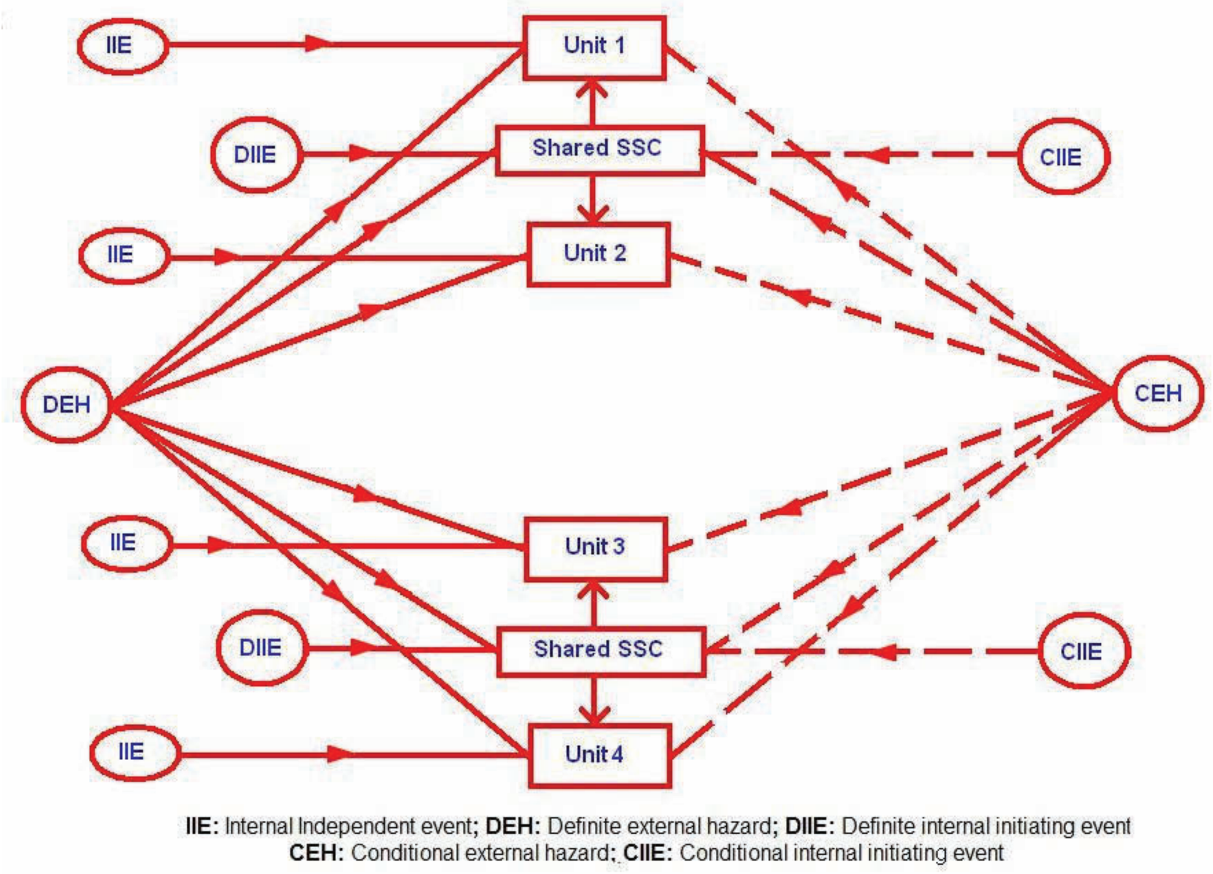


Fig. 3.2.7. Overall schematic for multi-unit safety assessment

Finally, in the last part of the research work "Integrated risk assessment for multi-unit NPP sites" is performed. Traditionally, a PSA is carried out to evaluate the risk associated with single unit NPP taking into account the defence in depth features and postulating combination of potential accident initiators for different hazards. But, a majority of nuclear power generating sites in the world houses more than one nuclear power plant. These sites are vulnerable to various hazards generated from external origin like earthquake, tsunami, flood, etc. which can jeopardise the safety of the plants. Further, the risk from a multiple unit site and its impact on the public and the environment was evident during the Fukushima nuclear disaster of March 2011. At present, there exists no established approach or methodology to estimate the risk from a multi-unit nuclear power plant site due to internal and external hazards. In the present work, an integrated approach is developed to assess the risk contribution of multiple nuclear plants at the site (Figure 1). The work highlights the importance of risks for multi-unit sites arising from shared system, common cause failures, failure correlations, cliff-edge effects, etc. from different hazards. Though the main emphasis on multi-unit safety is on external hazards, the proposed approach also includes risk from random internal events. The approach developed not only quantifies the frequency of multiple core damage for a multi unit site but also evaluates site core damage frequency which is the frequency of at least single core damage per site per year. Subsequently, the developed integrated approach is used to estimate and compare the risk from multi unit sites housing single, double, triple and quadruple nuclear plants. The developed approach is expected to be useful in developing safety goals, procedures and guidelines for a multi-unit NPP site.

The primary aim of the investigations carried out in the PhD was to study feasibility of activated flux gas tungsten arc welding (A-GTAW) process as alternate welding technique for naval structural steel (DMR-249A) and compare the effect of different arc welding processes on weld attributes of DMR-249A steel weld joints.

The experiments were carried out with combinations of oxide fluxes to develop suitable activated flux for GTAW of DMR-249A steel. The bead width and depth of penetration obtained in the bead on plate experiments using various combinations of fluxes were measured. Mixture 1, with maximum depth to width ratio about 0.86, was used as optimum flux combination to carry out experiments for optimising welding parameters for A-GTAW.

Four weld joints were fabricated using shielded metal arc welding (SMAW), submerged arc welding (SAW), flux cored arc welding (FCAW) and activated flux gas tungsten arc welding (A-GTAW) processes.

The Finite Element Model (FEM) simulation of thermo-mechanical behavior of SMAW (the most common welding technique used for welding of microalloyed steels and construction of ships) and A-GTAW (welding technique being studied and developed as alternative welding technique for DMR-249A steel) joints was studied using SYSWELD software. X-Ray Diffraction (XRD) and ultrasonic technique (UT) were used to experimentally estimate the residual stresses across the weld joints. The residual stresses profile of higher heat input A-GTAW process was observed to be comparable with SMAW process. A good agreement between measured and predicted thermal cycles and residual stress profile established FEM and UT as a dependable technique to estimate residual stresses in arc welded joints of DMR-249A steel.

The microstructure study of the base metal DMR 249A and the four weld joints were undertaken using optical microscope, SEM and EBSD (Fig.3.3.8). The microstructure of DMR-249A steel exhibited predominantly fine grained equiaxed ferrite and some percentage of pearlite of banded type structure. For weld metals, the optical micrographs showed grain boundary ferrite, Widmanstatten ferrite with aligned second phase along with veins of ferrite, acicular ferrite, polygonal ferrite and microphases. The minor changes in percentage of volume fraction of the different ferrites (grain boundary, Widmanstatten, acicular and polygonal) were observed in the samples characteristic to the difference in heat input of the various arc welding processes. The inclusion rating and estimation of volume fraction of various ferritic morphologies was undertaken to correlate microstructural transformation during welding with mechanical properties of various arc welded joints (Fig 3.3.8).

The hardness values measured across the weld joints were found within the scatter band of 200 -290 $HV_{0.2}$ as compared to values of 196-210 $HV_{0.2}$ for base metal. The tensile test performed on base metal and cross weld joint specimen showed higher yield strength about 460 - 480 MPa in the cross weld joints as compared to about 427 MPa of base metal (Table 3.3.1). The percentage elongation of cross weld joint (19-20%) was lower than the base metal (30%). The UTS of both the base metal and weld joints were comparable (about 600 MPa). The tensile fracture of the cross weld joint occurred in the base metal region away from weld metal which confirmed the existence of adequate strength in weld metal.The electrochemical properties of base metal (DMR-249A HSLA steel) and welded butt joints were compared by conducting potentiodynamic anodic polarization studies. It was concluded that the qualified arc welding processes did not deteriorate the corrosion characteristics of the base metal, DMR-249A steel.

Table 3.2.1 Comparison of tensile strength of DMR-249A steel and weld joints

Weld Joint	% Elongation		% RA	YS (MPa)	UTS (MPa)
	Uniform	Total			
DMR-249A	20	30	65	435	620
SMAW	12	20	63	480	610
SAW	10	17	63	450	595
FCAW	12	18	63	450	610
A-GTAW	13	20	63	480	640

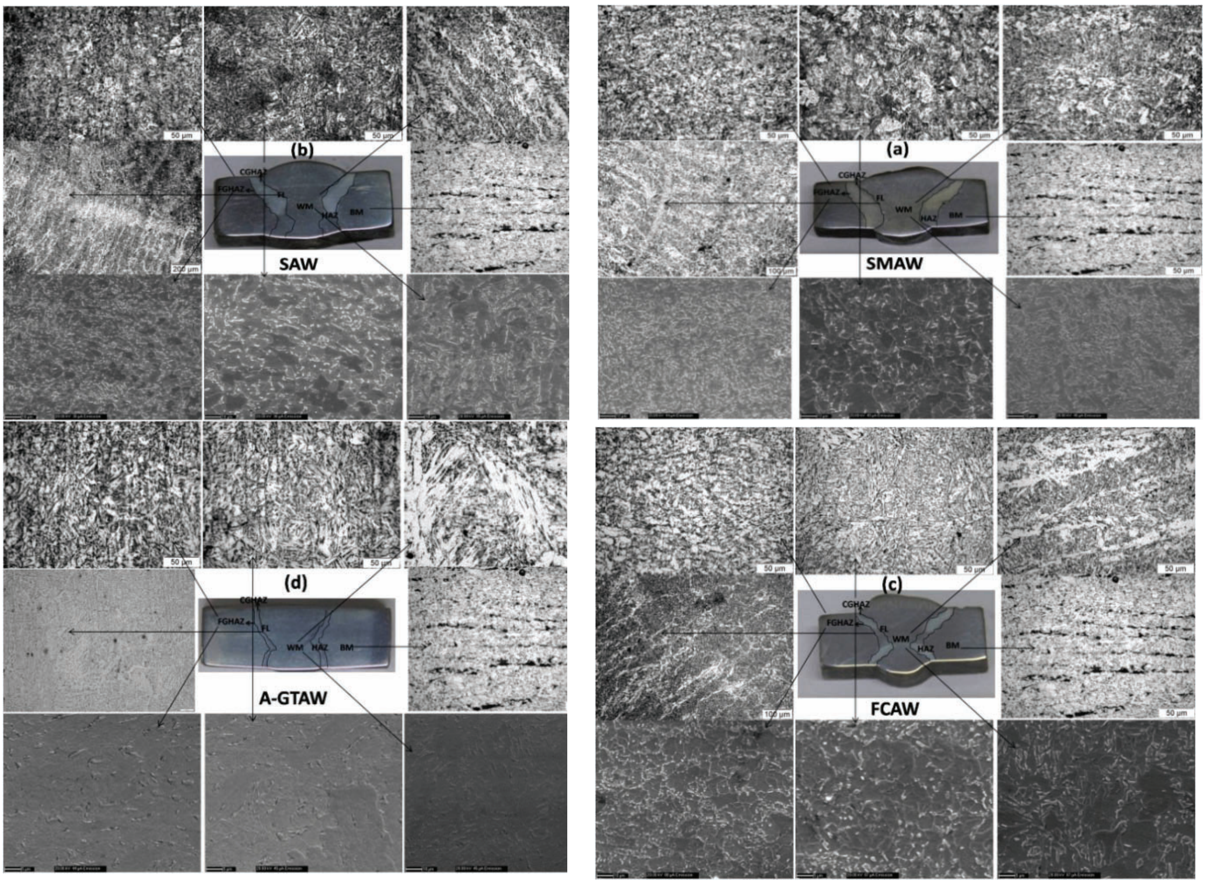


Fig. 3.2.8. Optical and SEM micrographs across the weld joints for SMAW, SAW, FCAW and A-GTAW joints

The impact toughness values of base metal (>350 J and 160 J respectively at room temperature and -60°C) was observed to be superior than the weld joints (160-200 J and 10-70 J respectively at room temperature and -60°C) (Table 2). The difference in impact toughness values is attributed to presence of impurities/inclusions in weld metal, coarse grain size due to welding heat input and traces of grain boundary and Widmanstatten ferrites in weld metal as compared to smaller equiaxed grains of base metal. The significant reduction in toughness of A-GTAW joint at sub-zero temperatures is attributable to more percentage of grain boundary ferrite and Widmanstatten ferrite in high heat input double pass A-GTAW welding process. The coarse grains of A-GTAW weld metal is also a significant factor leading to decrease in sub-zero impact toughness.

The weld attributes of phase transformation, microstructure, inclusions and mechanical properties were found to be distinctive characteristic of the different arc welding processes studied. The hardness, tensile properties and corrosion properties were found to be comparable for all the weld joints. The FCAW and SMAW joints exhibited better sub-zero impact toughness followed by SAW and A-GTAW. The significant variation observed in sub-zero impact toughness was attributed to the microstructral transformation of equiaxed base metal to various ferrite morphologies, grain size, inclusions and variation in chemical composition of weld metals of different joints.

Table 3.2.2 Comparison of impact toughness of DMR-249A steel and weld joints

Weld Joint	V-Notch Charpy Test			
	Room Temp (~25°C)		Sub-zero (-60°C)	
	Impact Toughness (J)	Lateral Expansion (mils)	Impact Toughness (J)	Lateral Expansion (mils)
DMR-249A	>350	110	155	110
SMAW	150	90	74	45
SAW	145	110	30	24
FCAW	210	110	50	40
A-GTAW	200	100	10	19

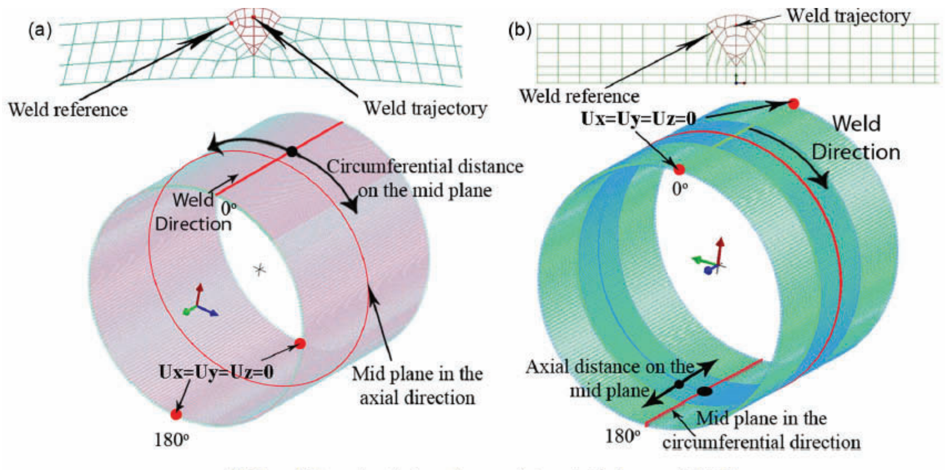
The experiments had been carried out with focus towards design and development of instrumented capsule for determination of uniaxial creep behavior in structural specimen. Analytical calculations and design have been carried out, the bellows setup has been fabricated through the industry. These bellows have been tested under cyclic load and found to be performing satisfactorily then fabricated an out-of-pile version of instrumented capsule. Argon at a pressure of 6.0 MPa has been filled in the capsule and sealed to apply a nominal load on the tensile specimen at room temperature. The instrumented capsule has been kept in the electric furnace and the temperature of furnace is raised. As the temperature of the furnace rises, the pressure of gas increases leading to increased load on the specimen. For validating the design concepts, these Experimental results have been compared with obtained literature results. Out-of-pile version of instrumented capsule has been designed and developed for online determination of uniaxial creep behavior in structural specimen.

Force/ load due to argon gas pressure is the major component for the tensile loading of the specimen. The 95% of the total load is acting on the specimen and remaining 5% load only is acting on the bellow. Experimental results (steady state creep values) have been compared with the literature results, and found to be closely matching. Design concept of instrumented capsule for uniaxial creep measurement has been validated. The design of instrumented capsule is directly applicable for in-reactor experiments of a fast reactor

Heat transfer analysis of irradiation capsule by analytical and simulation techniques have been carried out. In a nuclear reactor, structural material specimens are subjected to irradiation to determine the changes in their mechanical properties due to exposure to radiation. In one of the types of irradiation capsules, the specimens are kept in four to five separate sealed compartments of the capsule located one over the other. Helium/ Argon gas or mixture of these gases will be filled around the specimens in these compartments. Liquid sodium, which is the coolant in the reactor, will be flowing around the irradiation capsule. During irradiation, due to attenuation of gamma rays and neutrons on the specimens, heat will be generated in the specimens. Due to this, the temperature of the specimens will be more than the temperature of the sodium flowing over the capsule and we can obtain an irradiation temperature in the specimens which is higher than the sodium temperature. In the present analysis, the temperature of specimens has been determined with various types of gases (helium/ argon/ helium-argon mixture) filled in the compartment. Using the calculation methodology, the appropriate He-Ar gas mixture can be selected to obtain a desired irradiation temperature in the specimens.

Establishment of high temperature nicrobrazing procedure and qualification of brazed joints have been carried out . Fabrication of instrumented capsules requires the development of thin-walled joints capable of withstanding high temperatures. High-temperature brazing method has an advantage of joining multiple metal-sheathed cables such as thermocouples through a solid stainless steel plug in a single operation. High-temperature nicrobrazed joints under argon atmosphere have been produced as part of the project work. An induction heating technique has been used for this development. Protective atmosphere is required for high-temperature brazing to prevent oxidation of the base metal and the filler metal during the brazing operation. Commercial argon gas (99.996% pure) has been used and brazed joints have been developed. Brazing procedure has been established and development of high temperature nicrobrazed joints using induction heating in an argon gas environment has been done. Helium leak, metallographic, micro hardness tests, and sodium compatibility test have been carried out on the brazed samples.

Comparative study was carried out on weld joints developed by high temperature nicrobrazing, laser and GTAW joining processes. During assembly of an irradiation capsule, requires a weld joints at tube to end plugs. For this we need to optimize the parameters of available joining methods to qualify the tests according to the standards. Helium leak test, Metallographic and Micro hardness have been carried out on the joints made by laser, GTAW and high temperature nicrobrazing joining processes.

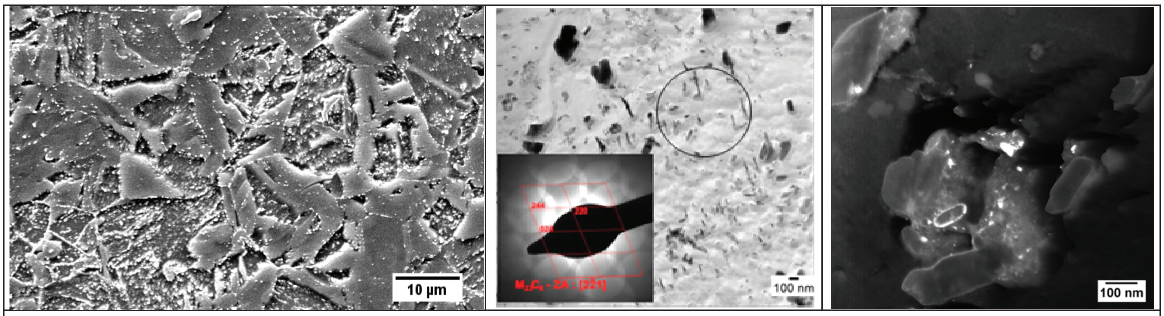


FE 2D and 3D mesh with boundary conditions: (a) L-Seam and (b) C-Seam.

An in-depth comparative study of different weld characteristics such as microstructures, physical properties, transient temperature distributions, residual stress fields and distortion patterns for different cases of axisymmetrical and non-axisymmetrical (N-A) butt welded joints has been carried out using a three dimensional sequentially coupled thermo-metallurgical-mechanical analysis; in order to improve the fatigue, stress corrosion cracking and fracture behaviour.Initially, weld experiments are performed to obtain the heat input and the macrographs which are further validated with the predicted weld molten pool sizes during Heat Source Fitting (HSF) analysis. The Goldak's double ellipsoid heat source function obtained in HSF analysis is employed in the thermal and mechanical analysis.In this investigation, the effectiveness of the developed finite element simulation strategy is verified by validating with the experimental weld characteristics.

There are significant differences in 3-D temperature profiles, temperature distributions and residual stress states between L-Seam and C-Seam butt joints; and run and branch pipes of BP-T-joints for different pipe sizes along different sections. Residual stress distributions for the three plane axisymmetrical butt weld joint are investigated and their effects on the CE rotating bowl are discussed.The major findings of this investigation are: (i) L-Seam weld joints are not advisable to use while fabricating cylindrical components in order to improve the service life; (ii) joining of branch pipes to run pipes by using a single N-A butt weld joint is the most successful method instead of three circumferential axisymmetrical butt weld joints.

The thesis has brought out an in-depth understanding on various aspects of two variants of RAFM steels with 1 and 1.4 weight% of tungsten, which have been indigenously developed as structural materials for the plasma facing Test Blanket Module in fusion reactors. The effect W on the microstructural evolution during various thermal treatments and welding has been studied in detail with respect to prior austenite, lath size and microchemistry of secondary phases in the two steels as a function of time temperature which is important as far as the stability of steel is concerned. The creep and toughness properties were evaluated employing two innovative small specimen testing methods namely impression creep and automated ball indentation techniques. These studies have clearly established the role of W in enhancing the creep strength both in terms of solid solution strengthening and stabilizing the microstructure as well as the degradation of toughness on aging due to formation of detrimental Laves phase.



TEM micrographs showing a) mixed microstructure consisting martensite and ferrite in the Intercritical HAZ of RAFM weld b) presence of fine needle type fe rich precipites in the weld metal after aging at 773K/5h c) Dark field image of Laves phase surrounding coarse carbide, after aging at 833K/5kh

The heterogeneous microstructure in the weld HAZ as function of thermal cycles has not only been studied using a variety of electron microscopy techniques but also been validated by GLEEBLE test. The influence of PWHT as well as long term aging on the microstructure and secondary phases has been systematically investigated and the role of prior microstructure on the kinetics of secondary phase evolution has been established. Additionally, the microstructures that evolve in a 316L-RAFM dissimilar weld joint due to mixing and dilution has been studied. Formation of delta ferrite at the austenite boundary and the austenite-ferrite mixed microstructure in the weld due to diffusion of Ni has been established using the state of art EBSD technique. The effect of Ni diffusion on the transformation characteristics of RAFM steel has been demonstrated using Differential Scanning Calorimetry and computational methods. The highlights of the thesis includes:-

- Microstructural evolution of welded joints of INRAFM steel
- Precipitation of Laves phase in INRAFM steel on prolonged thermal exposures
- Early precipitation of Laves phase in FGHAZ is due to the accelerated carbide precipitation kinetics assisted by the thermal cycle experienced in the zone
- Optimization of PWHT conditions for indigenous RAFM steel

3.3 Variable Energy Cyclotron Centre (VECC), Kolkata

During the period, 3 students were awarded Ph.D. degree in Engineering Sciences. Highlights from some the theses are presented as follows.

The present research aims to devise a novel scheme for DSP based power converter coupled to a Superconducting Magnetic Energy Storage (SMES) system to mitigate voltage sags originating in the utility mains so as to keep the load voltage free of any interruptions. The associated control philosophy is based on correctly identifying the voltage sag in the AC utility lines and efficiently compensating it, both in amplitude and phase, by appropriately switching the power devices. Based on the schemes presented in various literatures, the selection of the proposed (Fig. 3.4.1) Dynamic Voltage Restorer (DVR) scheme was justified.

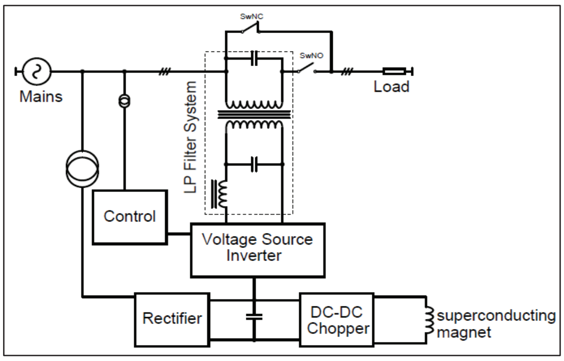


Fig. 3.3.1: The SMES based DVR

A digital control system was designed for the Voltage Source Inverter (VSI) stage that utilized a Software Phase Locked Loop (SPLL) for phase locking and voltage sag detection. A fixed point DSP based controller was programmed to implement the same besides generating Space Vector Pulse Width Modulation (SVPWM) switchings and handshaking between the subsystems of the integrated DVR.

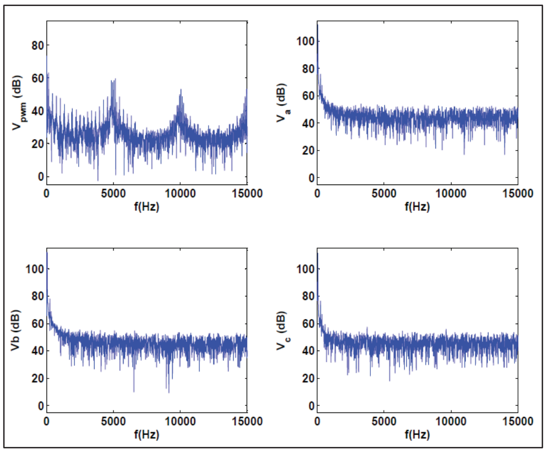


Fig. 3.3.2: Harmonics at the PWM signal (top left) and those at load phases

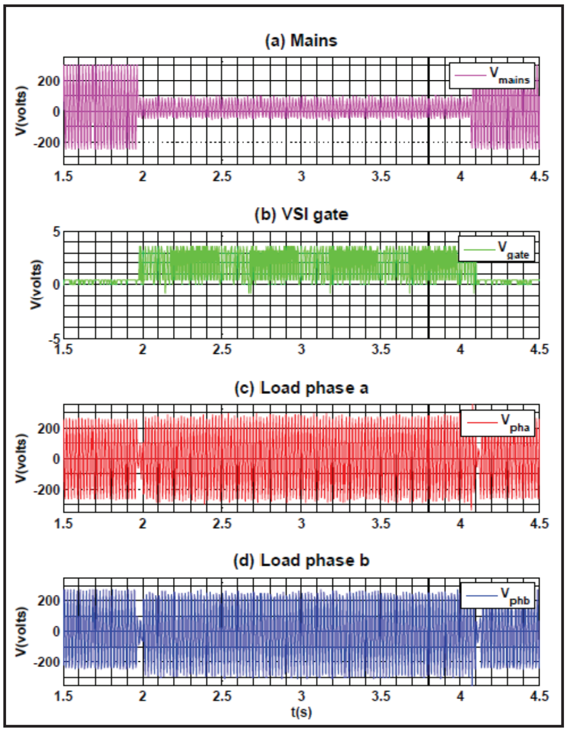


Fig. 3.3.3: (a) A voltage sag occurs at mains and is restored after more than 2 sec, (b) the controller initiates gate triggering of VSI, (c), (d) the load phases maintaining the same voltage within 2 cycle

A novel low pass filter scheme for the VSI was presented based on a set of performance indices reflecting the quality of the filter and the ratings of the filter components. In the process, an attenuation of 60 dB was achieved (Fig. 3.4.2). The design was kept generalized so that it may be applied on any VSI system.

The VSI was configured for SMES based DVR for a 3- 240 V, 50 Hz, 3.45 kW load for voltage sag mitigation according to IEEE 1159-1995. Voltage sags of varying depths were mitigated for 40 ms to 6 sec with phase locking. This demonstrated the system's performance for satisfactory phase locking and voltage compensations (Fig. 3.4.3) for momentary sags and partly for instantaneous and temporary sags.

A necessary prerequisite for autonomous navigation of mobile robots is the capabilityof localization. If a map of the environment is available with the robot *a priori*,it will be able to localize itself by matching its perception of the environment with the map. However, the processes of automatic map building and that of localization are closely intertwined. Hence,they are usually solved concurrently, using methods commonly known as *Simultaneous Localization and Mapping* (SLAM).But, in many real-life applications, it is more appropriate to build a map of the working environment first and then use it for localization, rather than operate the robot in online SLAM mode, which is complex, computation-intensive and less accurate.

With the objective of achieving robust and accurate localization of mobile robots equipped with a laser range finder in indoor environments that practically remains invariant over extended periods of time, in the thesis, we propose

- an offline method for building maps of indoor environments by merging line segments extracted from registered laser range scans; and
- a robust and accurate method for localization on such maps based on the Monte Carlo framework.

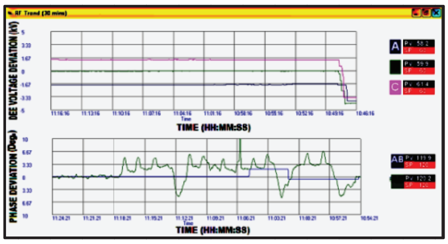
Line segments are a natural choice in the representation of indoor environments. Maps based on line segments are compact, provide floating-point resolutionand scale well with the environment size. The proposed method has been successful in accurately building maps of large environments from datasets available in the public domain as well as from simulated and real-world data. Experimental results show that maps produced by the proposed method are generally better than those produced by two other methods reported in the literature in terms of compactness and accuracy.

Monte Carlo Localization (MCL) is a powerful and popular approach for mobile robot localization. But MCL has seldom been studied in the context of linesegment-based maps. A key step of the approach is the computation of the so called *importance weight* associated with each hypothesized pose or particle.In the thesis, we propose a novel, heuristic-driven approach for the computationof importance weights in MCL on maps represented with line segments, and extensivelystudy its performance in pose tracking. We also compare our method with three othermethods reported in the literature. The comparative study, conducted using bothsimulated and real data, on maps built from real data available in the public domainclearly establish that the proposed method is more accurate, robust and efficient thanthe other methods.

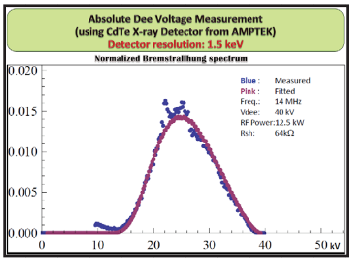
In the concluding part of the thesis, we point out several open issues for further research. In the backdrop of what has been presented in the earlier part of the thesis, we discuss on a probable way to achieve added robustness and accuracy in localizationson as to make the proposed methods of map building and localization more useful and efficacious for deployment in real-life applications.

The dissertation discussed thoroughly the electromagnetic modeling and simulations, design and analysis of room-temperature coaxial type large cavities for the K500 Superconducting cyclotron. The coarse and fine tuning system has been designed and developed for the above machine.

An indirect method using continuous X-ray spectrum has been employed to measure absolute RF voltage at the accelerating gap of the cavity within ± 1.5 kV. The automatic phase control system has been designed and developed to achieve phase stability within ±0.1 degree between any two cavities, under continuous high power operation of the K500 cyclotron. This phase control system has a special design feature of having both analog in-phase/quadrature (I/Q) modulator based phase regulator and Direct Digital Synthesis (DDS) based phase shifter in order to achieve faster response along with wide dynamic range (±180 degree) as well. Also, high power RF amplifier has been designed and developed for feeding power to the K500 superconducting cyclotron.



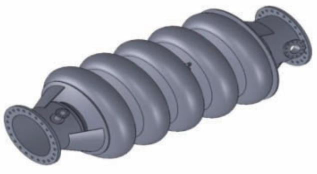
Phase stability (Bottom Plot) for 30 minutes where. AB phase loop was CLOSED, AC loop was OPEN



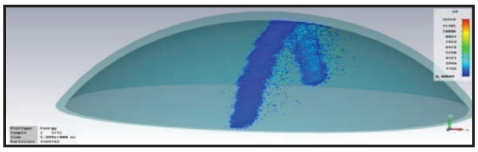
Measured X-ray Spectra at 40kV dee Voltage at 14 MHz

A new electromagnetic design of five-cell elliptical superconducting RF cavity operating at 650 MHz in $\beta = 0.61$ region for the proposed 1GeV, 2mA proton linear accelerator, has been carried to achieve accelerating gradient of 17 MV/m. The cavity design offered some new features, comprising of wide aperture (96 mm) for better acceptance and moderate value of wall slope angle (2.4 degree for mid cells and 4.5 degree for end cells) for better mechanical rigidity and also better accessibility for surface processing.

Although 2D study shows hardly any possibility of multipacting, the 3D multipacting study and analysis based on Furman model with due consideration of three kinds of secondary electron emissions – true secondary, elastic back scattered secondary and rediffused secondary electrons, for 650 MHz, $\beta = 0.61$, SRF cavity, shows possibility of multipacting within a specific electric fields. Besides true secondary electrons, the elastic back scattered and rediffused secondary electrons, are also responsible for the multipacting at the electric fields between 5.8 MV/m and 11.5 MV/m in the above cavity. There is no possibility of multipacting below 4.5 MV/m and above 22.5 MV/m.



Iosmetric view of 5-cell SRF cavity



Particle growth at the equator region of the cavity after 6 ns at accelerating gradient of 6.8 MV/m (using 3D CST Particle Studio)

The research issues for further development are wide open for room temperature cavities and also for superconducting cavities, in terms of achieving higher and higher accelerating gradients. The on-going progress in the development of new cavity materials will definitely improve the performance of the cavities. The continuously developing and upgraded manufacturing and fabrication processes and also improved measurement techniques have the scope of achieving better performance of the cavity and its associated controls. The design of LLRF controller, especially, the high stability phase controller, as discussed in the thesis, has a great scope of utilization in any high power accelerator cavities.

Department of Atomic Energy is considering a high intensity accelerator to deliver a 1 GeV, 10 mA proton beam for Accelerator Driven Subcritical System. As a first step towards the development of this system, a R&D program is underway at Variable Energy Cyclotron Centre for the development of 2.45 GHz proton source along with a low energy beam transport system (LEBT) to study the production and transport of proton beam in the range of (10-15) mA at ~75 keV energy. At present, the ion source is operational and produces a 12 mA beam current for 400 W of microwave power. A beam current of ~ 6 mA through a 10 mm diameter aperture has been transported to three meters from the ion source.

In this research, we present a detailed study investigating the effect of variation in different parameters of the ion source, like, for instance, microwave power, magnetic field profile, gas pressure, etc. on the performance of ion source. It is demonstrated that these parameters have significant impact on the extracted beam current and proton fraction. This research work also presents a unique analytical method for the design of binomial matching transformer. A comparison of the results obtained from analytical method and finite element method simulations, shows that they are in good agreement. It is demonstrated that usage of optimum matching transformer improves the performance of microwave ion source. The maximum beam transmission and the beam quality in LEBT are limited by the space charge effects of high current proton beam. Thus, these effects must be mitigated by space charge compensation (SCC). The compensated beam should also be characterized before injecting it into the cyclotron. This research work reports the results of SCC in a 75 keV, 5mA proton beam. The SCC is realized by injection of Ne gas into the beam line. It is shown that RMS beam size reduces by ~ 34 % with the SCC. A residual gas fluorescence monitor was designed to measure the beam profile.The solenoid scan with sigma matrix method was used to determine the normalized RMS beam emittance. It is measured to be of 0.05 mm-mrad, which is within the requirement of all upcoming high intensity accelerators.

4. Life Sciences

During this period, HBNI awarded Ph.D. degree to 38 students who carried out research in the area of Life Sciences at different CI/OCC of HBNI. Highlights of research specific to different CIs are as follows.

4.1 Bhabha Atomic Research Centre (BARC), Mumbai

In the period from April 2016-March 2017, nine students were awarded their Ph. D. degree in Life Sciences in BARC in varied topics ranging from bacteria to animal and human cells.

The highly radioresistant bacterium *Deinococcus radiodurans* was genetically modified to aid in the precipitation of uranium over a wide pH range from acidic to alkaline conditions, by overexpressing the acid (PhoN) or alkaline (PhoK) phosphatase genes. Cell-associated precipitate was observed at acidic pH while extracellular precipitate was observed at alkaline pH, the precipitated uranium identified as chernikovite (Fig. 4.1.1).

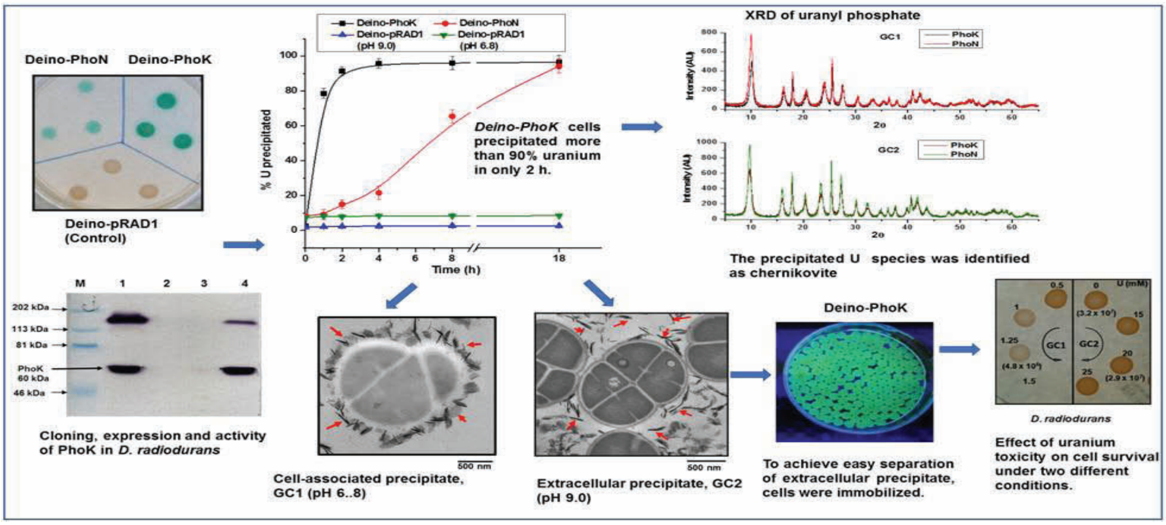


Fig. 4.1.1. Bioremediation of uranium from acidic and alkaline solutions using genetically engineered Deinococcus radiodurans

The promoters regulating the expression of genes in *D. radiodurans* were characterised using several radiation-inducible promoters as test system and fluorescence (GFP) based reporter assay system. This helped identify a *cis*-regulatory element (RDRM) placed close to the promoter region, regulated by a proteolytically cleavable regulatory protein DdrO as shown in Fig. 4.1.2.

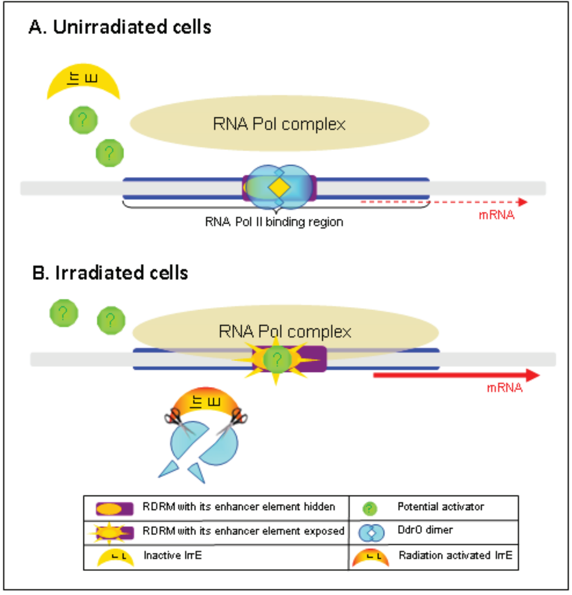


Fig. 4.1.2. A model for gene regulation by DdrO-RDRM-PprI-RNA pol

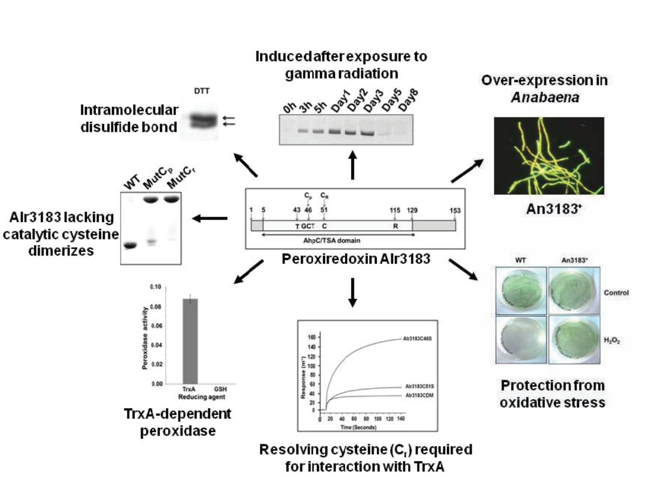


Fig. 4.1.3. Characterization of peroxiredon Alr3813 from Anabaena PCC7120

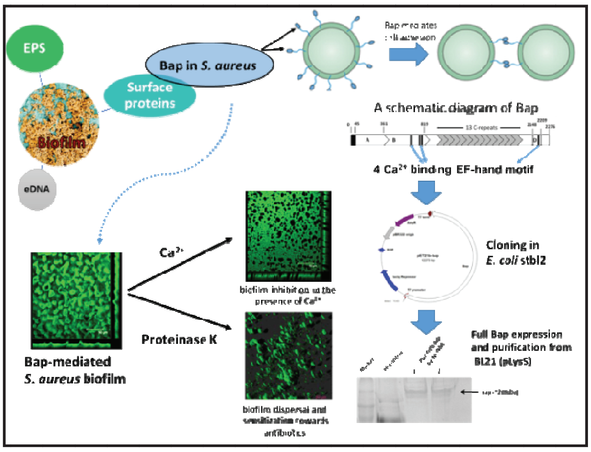


Fig. 4.1.4. Molecular studies of biofilm-associated proteins of Staphylococcus aureus.

Tolerance to radiation stress also requires the organism to be able to overcome oxidative stress by effectively removing the ROS. The peroxiredoxin, Alr3183 of the cyanobacterium, *Anabaena* PCC7120 induced under radiation stress effectively removes ROS and thereby enhances the oxidative stress tolerance of the cyanobacterium. This was characterised as a monomeric TrxA-dependent peroxidase.

Bacteria contribute to biofilm formation which is a serious health concern and a major cause for persistent infections. The bacterium *Staphylococcus* sp. is notorious for biofilm formation. The proteins involved in biofilm formation in *S. aureus* were investigated. Bap-mediated biofilm formation was investigated (Fig. 4) with a potential use for developing methods for control of persistence in infections and biofouling of cooling water plants.

Radiation, when used at a specified dose and with targeting, can be used to cure cancers. But, unlimited/accidental exposure could give rise to several genetic mutations, including those inducing cancer. However, the population living in the high level natural radiation areas (HLNRA) in the coast of Kerala, India exhibit no significant increase in abnormalities or cancer incidences compared to those living in normal areas. Based on biological end point studies such as DNA repair, gene expression analysis and conformational changes in chromatin, it was concluded that the chronic low level exposure to radiation enhances the capability of DNA repair contributing to low mutation rates and cell death.

The cure of cancer is an important area of research with increasing focus on natural drugs rather than chemically synthesised drugs for chemotherapy. One such drug is malabaricone C (mal C) derived from Rampatri. Mal C exhibited higher cytotoxicity than curcumin as well as etopiside contributed by its pro-apoptotic action (Fig. 4.1.5). Thus, mal C could serve as a chemotherapeutic agent for cancer especially in tumours lacking caspase-3 activity. Mal C could remodel the cardiovascular properties by modulating the cardiac structural and functional parameters in mice. Thus, it could also be used as a potential non-toxic drug for treatment of cardiovascular diseases.

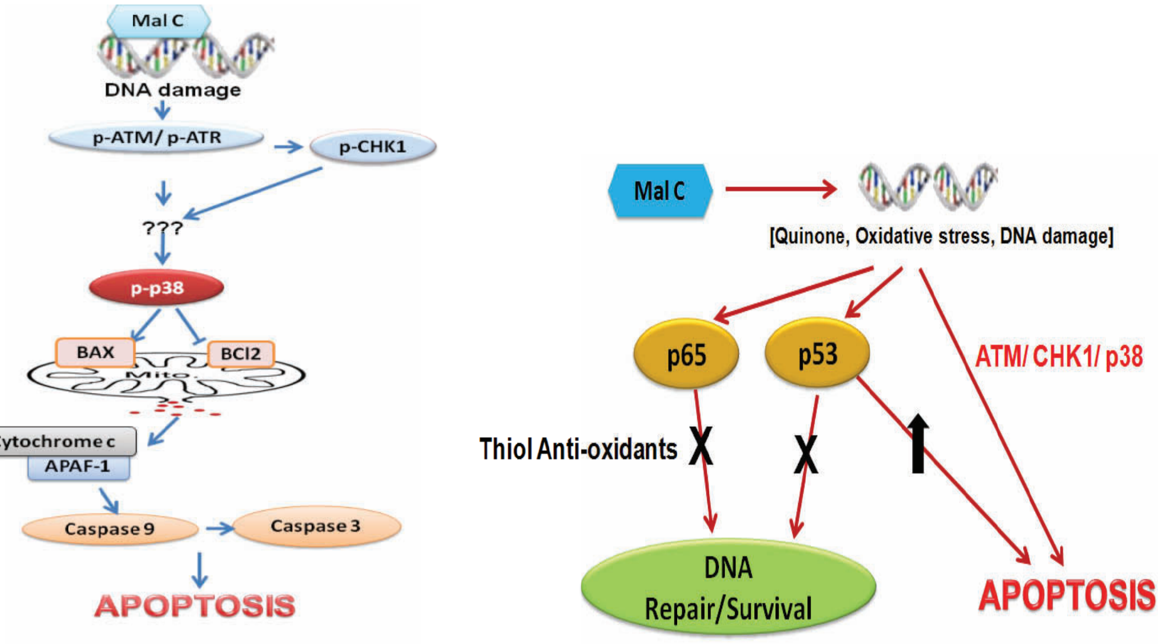


Fig. 4.1.5. Model depicting the pro-apoptotic activity of malabaricone C

Another potential therapeutic agent is the plant derived flavonoid, baicalein. When tested using murine splenic lymphocytes, it exhibited radioprotective properties. A mechanistic evaluation of its function revealed that baiclaein acts through activation of NF-κB and blocked the thioredoxin activity (Fig. 4.1.6), thus increasing the radiosensitivity of the tumor, and acting as an anti-tumor drug.

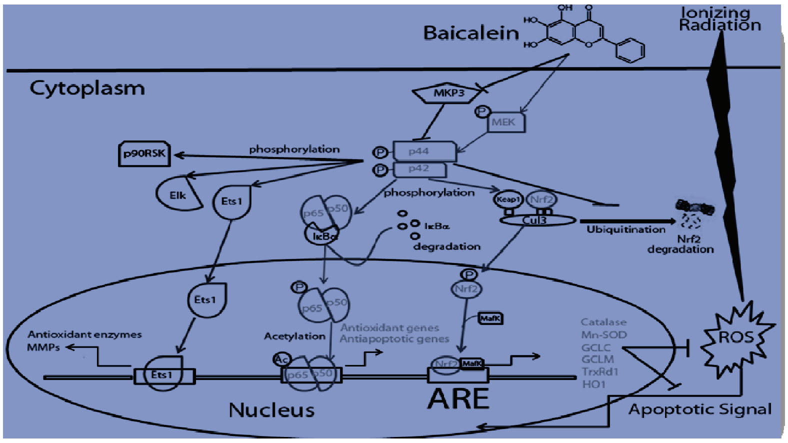


Fig. 4.1.6 Mechanistic action of Baicalein

Multianalyte immunoassay (MAIA) is the need of the day to cover large sample sizes and rapid detection of diseases. Using thyroid diagnosis as a model, MAIA was developed for Thyroxine (T4), thyroid stimulating hormone (TSH) and thyroglobulin (Tg) as shown in Fig. 4.1.7. ^{125}I labelled antigens/antibodies were used and a microporous polycarbonate track-etched membrane (PC-TEM) was found to be an excellent and novel support for antibody-chip production. Validation of all QC parameters for immunoassays, the MAIA by the virtue of miniaturized assay format can save on assay time, costs and patients' sample required.

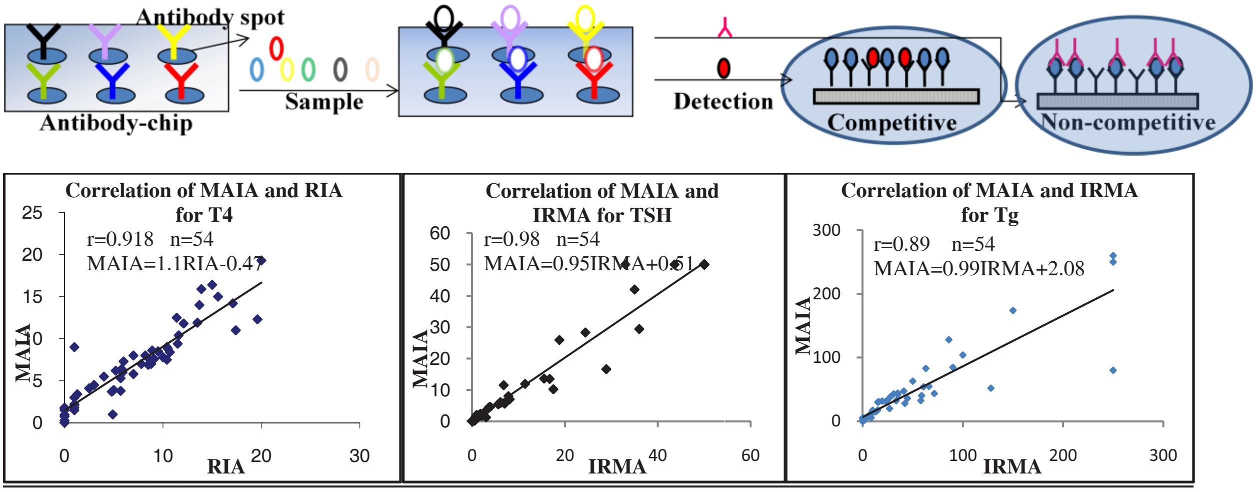


Fig. 4.1.7. Schematic illustration of principle of MAIA and comparison of T4, TSH and Tg concentration in human serum samples measured by MAIA & RIA/IRMA

4.2 Raja Ramanna Centre for Advanced Technology (RRCAT), Indore

Thesis devoted to the study of effect of topical antimicrobial photodynamic treatment (APDT) mediated by poly-L-lysin conjugate of chlorine p6 (pl-cp6) on healing of wounds. Important result presented in this thesis includes demonstration of photobactericidal efficacy of pl-cp6 is higher than free cp6 and phototoxicityinduced by pl-cp6 is more selective to bacteria than host cells.Studies on influence of pl-cp6 mediated topical APDT on the healing and inflammation of P. aeruginosa infected wounds in mice showed that APDT, apart from reducing bacterial load, also leads to attenuation of the infection induced hyperinflammtory response of wounds. It was also shown that APDT leads to not only reduction of wound bacteria number but also attenuation of infection induced inflammation, improved angiogenesis, enhanced collagen remodeling while avoiding damage to host inflammatory cells.

4.3 Tata Memorial Centre (TMC), Mumbai

Advanced Centre for Treatment, Research & Education in Cancer (ACTREC), TMC is a comprehensive Cancer Centre dedicated to cancer research and patient care. The Institute offers PhD (Life Science) degrees and is affiliated to Homi Bhabha National Institute (HBNI). The following is a summary of 23 PhD theses submitted to HBNI under various areas of Cancer Biology in 2016-17.

Stem Cell Biology and Cell signaling

Ovarian cancer is the 7th most common cancer amongst women and ranks 4th in cancer related deaths across the globe. In the Indian scenario, it is the 4th most common cancer amongst women. Generation of chemoresistance and relapse are the major hurdle in the disease management. In the present thesis, we found an enrichment of SP fraction with increased self-renewal and stemness phenotype during acquirement of resistance against cisplatin, paclitaxel and combination treatment in ovarian cancer cells. Real time monitoring of tumor formation with bioluminescence imaging showed that SP cells from Pac^{ER} stage initiated tumor formation much earlier than SP cells from Cis^{LR} stage suggesting functional heterogeneity within CSCs. We also reported a preferential regulation of IGF-1R and AKT signaling at early and late resistant stages respectively. While IGF-1R levels were found to be up regulated only at early stages (Cis^{ER}, Pac^{ER} and Cis-Pac^{ER}), higher levels of activated Akt was associated with late resistance. Inhibition of IGF-1R expression resulted in down regulation of stemness like phenotype and stemness gene expression. Thus it is probable that higher IGF-1R expression is required for initiation of resistance development along with maintenance of the CSC like phenotype. Using small molecule inhibitors against IGF-1R auto phosphorylation, we showed increased potentiating cytotoxic effects of chemotherapeutic agents at early stage of resistance. As IGF-1R levels go down in late resistant cells (CisLR, PacLR and Cis-PacLR), it is possible that high level of pAKT maintains chemoresistance and CSC like phenotype. It would be interesting to identify the transcriptional regulators of IGF-1R and AKT signaling and understand the relation between stemness genes and IGF-1R/Akt signaling at early and late resistant stages in the future.

Protein Biochemistry, Biophysics & Structural Biology

BRCA1-BARD1 E3 ubiquitin ligase and CstF50 protein-protein complex play an important role in transcription coupled DNA damage repair. Germ-line mutations identified in BARD1 ARD-BRCT linker region at Gln564His position impaired complex formation between BARD1 and CstF50, which in turn led to premature transcript formation, uncontrolled mRNA regulation and reduced apoptosis. Biophysical and in-vitro assays could unravel the changes in folding pattern and structural integrity of the BARD1 *wild-type* and Gln564His mutant protein. Molecular docking studies of CstF50 with BARD1 *wild-type* and mutant showed loss of weak intermolecular interactions in mutant protein. Molecular dynamics simulation showed that mutant protein was more dynamic in nature compared to *wild-type* protein*.* It was observed that the C-terminal domain of BARD1 was an evolutionarily conserved phosphopeptide binding domain and had a wide role to play in DNA damage repair (DDR) and cell-cycle regulation. Cancer predisposing mutations C645R, R658C, V695L, I738V and S761N are reported in BARD1BRCT domain. Thermal and chemical denaturation studies revealed a decrease in the thermodynamic stability of BARD1 V695L, S761N, R658C and I738V mutants as compared to the *wild-type,* and all the proteins unfolded via intermediate formation. Molecular dynamics simulation studies of *wild-type* and mutant protein structures indicated that the mutants had lost structural integrity as compared to the *wild-type* protein. We also described the inhibitory effect of platinum drug on E3 ubiquitin ligase activity of BRCA1-BARD1 Ring domain complex. The docking study between platinum drug and BRCA1 Ring domain showed the overlapping of platinum drug binding site with E2 ligase binding site; this led us to conclude that platinum drug might interfere with E2 binding. Multidisciplinary comparative studies of BARD1 *wild-type* and mutants would be helpful in understanding the role of BARD1BRCT in DDR, cell-cycle regulation and tumorigenesis.

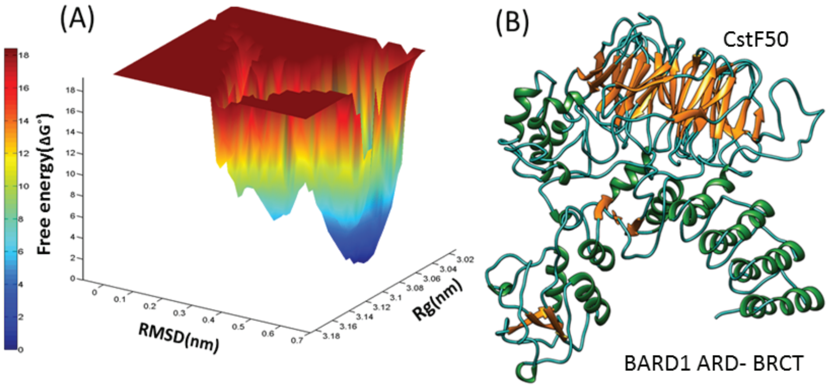


Fig. 4.3.1. BARD1 ARD-BRCT wild-type CstF50 complex; (A) Free-energy calculation (B) Representative structure of the BARD1 ARD BRCT – CstF50 complex

Cancer is a disease caused by mutations on signaling proteins, thereby deregulating several metabolic pathways. MAP kinase (MAPK) pathway, involving several proteins, is severely deregulated in many known human cancers. The signaling proteins such as extracellular signal regulated kinases and ribosomal S6 kinases play a major role in cell signaling. Considering the importance of MAPK pathway, structural, biophysical and protein-protein interactions of different domains of kinases proteins were reported in this thesis. Various techniques such as molecular cloning, protein purification, proteomics, biophysical characterization and bioinformatics were extensively used to fulfil the objectives set for the Ph.D. thesis. ERK 2 was purified to study the protein-protein interactions with binding proteins. ITC was used to quantity the interactions with RSK 3 C terminal synthetic peptide. Further, protein-protein interactions studies between ERK2 and MEK1, ERK2 and RSK1 were studied using in-silico molecular docking. Docking studies were performed between ERK2 and C terminal peptides of all RSK 1/2/3/4 isoforms. RSK1 full length protein of 735 amino acids was purified and studied for its biophysical properties. It was observed that RSK1 was α-helical in nature, however less stable due to its lower T_m. RSK1 CTKD (418-675) was cloned and expressed, and purified from inclusion bodies under denaturing conditions using 8 M urea. Furthermore, RSK3 NTKD and CTKD were cloned, expressed and purified under denaturing conditions as they were insoluble. RSK3 CTKD was successfully refolded after screening large number of buffers by trial and error. The refolded RSK3 CTKD was further characterized by various biophysical techniques such as fluorescence spectroscopy, CD, limited proteolysis. It was found that the RSK3 CTKD was rich in α-helical content and stable due to high T_m and slow rate of proteolysis. Further DLS studies proved that RSK3 CTKD existed as a trimer in solution. Overall this study further strengthened the understanding of function of MAPK pathways in cell signaling with an emphasis on ERK2 and RSKs, through different biophysical and bioinformatics studies.

HtrA2, a trimeric proapoptotic serine protease plays pivotal role in maintaining cellular homeostasis by mediating apoptosis via multiple pathways. Differential expression of HtrA2 has been associated with neurodegenerative diseases, hepatocellular carcinoma as well as cancers such as ovarian, breast and prostate, thus making it an important therapeutic target. Upon substrate binding, this protein regulates its functions through coordinated conformational changes, the mechanism of which is yet to be elucidated. Most of its cytoplasmic partners and substrates such as IAPs, Pag, Mxi-2 and Pea-15 [6, 7-8] suggest an interaction after being released from the mitochondria. However, subsequent studies have identified a mitochondrial anti-apoptotic protein HAX1 (hematopoietic cell specific Lyn-substrate 1) as a binding partner cum substrate of HtrA2, which on interaction with the latter degrades and leads to subsequent activation of HtrA2 as an early event in apoptosis [9]. However, details of this interacting complex and mechanism of action are yet to be delineated.

Although allostery has been found in some of its homologs, it has not been very well characterized in HtrA2. Our *in silico* studies led to prediction of the putative binding pocket which together with modeling, molecular dynamics simulation, enzymology and other biochemical studies helped us identify and demonstrate its role in allosteric regulation of HtrA2 activity. This non-classical binding pocket is unique among HtrA family proteins and thus unfolds a novel mechanism of regulation of HtrA2 activity and hence apoptosis. In the cellular scenario, the allosteric mechanism is of significance for HtrA2 regulation by its binding partners and vice-versa. Hence, the other part of our study was to elucidate the mechanism of intrinsic pathway of apoptosis in context of HtrA2 and one of its key interacting partners in the mitochondria, HAX1.

HAX1 is a ubiquitously expressing anti-apoptotic protein that regulates mitochondrial membrane potential. Despite suggestions of its involvement in a novel alternate apoptotic pathway, the structural details, stoichiometry and mechanism of HtrA2-HAX-1 interaction and subsequent event in the mitochondria are yet to be elucidated. Our *in silico* interaction studies and *in vitro* pull down assays provided information on interacting domains, the minimal binding region and the critical residues involved. With comprehensive enzymology studies we also provided evidence demonstrating for the first time that HAX1 is an activator of HtrA2 - which could prove to be a critical step driving early stages of apoptosis. The other players in the complex mechanism were also taken into consideration for better insights in the mechanism. These studies put together helped us design allosteric peptide modulators that might be an excellent approach to modulate HtrA2 functions. The peptide based approach exhibited several advantages over conventional orthosteric molecules, such as low toxicity and higher subtype specificity.

These findings could thus be utilized for designing small molecule inhibitors in therapeutic strategies against cancer and other diseases.

While trying to understand the domain architecture and roles of different domains in HtrA2, we realized the importance of the PDZ domain both in the functional dynamics of the protein as well as protein-protein interactions. Surprisingly there was not a single database with updated information on this important class of PDZ containing proteins and their interacting partners. With an aim at providing updated and comprehensive information on these proteins, we developed a PDZ domain database, 'PDZome,' that comprises details of 42,043 proteins and their interacting partners. This would be of great value to both basic and clinical researchers in this field both for identifying new targets as well as establishing therapeutic strategies.

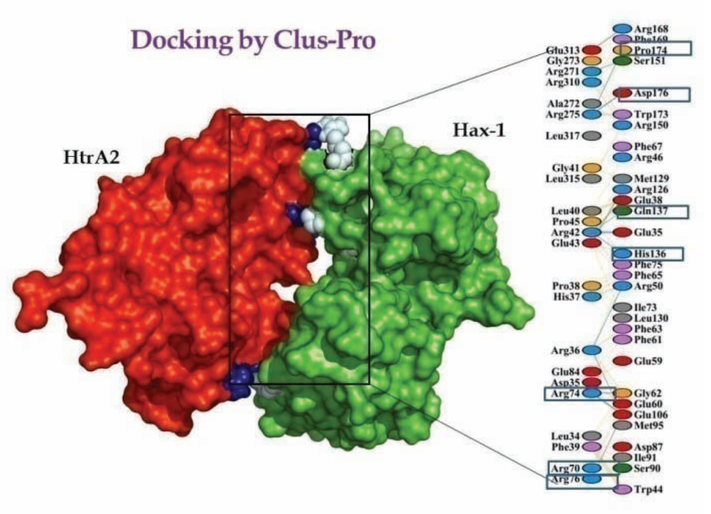


Fig. 4.3.2 Critical residues for interaction between HtrA2 and HAX-1 as identified by Clus-Pro software

Cancer Epigenetics

Histones are a class of highly conserved basic proteins and packaging the genome was the primary function previously attributed to them. The core histones comprise of H2A, H2B, H3 and H4 which assemble as hetero-oligomers to form the octameric protein core of the fundamental repeating unit of chromatin, the nucleosome.

Histone genes are present in clusters and in multiple copies. For instance, in humans, H2A is coded by 16 genes. All of these genes do not code for the identical protein and give rise to sequence divergent forms of histones termed isoforms. H2A isoforms are known to exhibit altered expression under different physiological conditions. Their distinct functional effects remain a matter of investigation and the mechanistic basis of the non-redundancy is elusive.

Here, we showed that isoform H2A.1 exhibits drastically altered expression pattern in normal tissues and cancer cells. It is of functional importance as H2A.1 promotes cell proliferation in a context dependent manner. For carrying out comparative analysis of the stability of H2A.1 and H2A.2 containing nucleosome and sub-nucleosomal complexes *in vitro*, the histone proteins were recombinantly purified. Further, sub-nucleosomal complexes were reconstituted and purified. Biophysical characterization showed that M51L alteration at the dimer interface decreases the temperature of melting of H2A.1-H2B by ~3^0C as compared to H2A.2-H2B dimer. Further, M51L and K99R substitutions made H2A.1 containing nucleosomes more stable by increasing the number of hydrogen bonds and hydrophobic interactions. Interestingly, the same two substitutions had the most prominent effect on cell proliferation suggesting that the nucleosome stability is intimately linked with the physiological effects observed.

In summary, the incorporation of the histone isoform H2A.1 resulted in increased nucleosome stability, which is expected to contribute to the contextual alteration in global transcription pattern and other chromatin mediated processes.

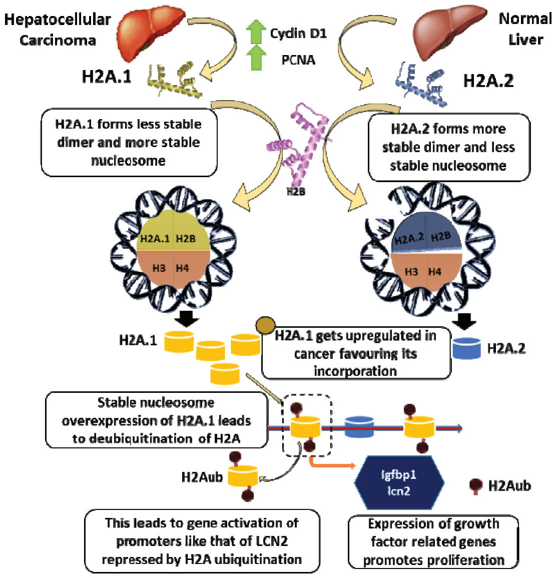


Fig. 4.3.3. Histone H2A.1 Promotes Attainment of Distinct Physiological States by Altering Chromatin Dynamics in hepatocellular carcinoma

Cancer Cell Biology

Dissemination of cells from primary tumor to secondary non-contiguous site is called metastasis. Despite of high death rate in cancer patients is due to metastasis, it is poorly understood because of its complexity and multistep nature. Cell surface molecules play a crucial role in all the steps of metastatic cascade. Tumor cells show several cell surface modifications associated with the metastatic phenotype, including changes in the cell surface glycosylation.Previous work in the lab had shown that polyLacNAc substituted β1, 6 branched N-oligosaccharides expressed on B16F10 promoted lung specific metastasis via galectin-3 which was expressed in highest amounts on the lungs.

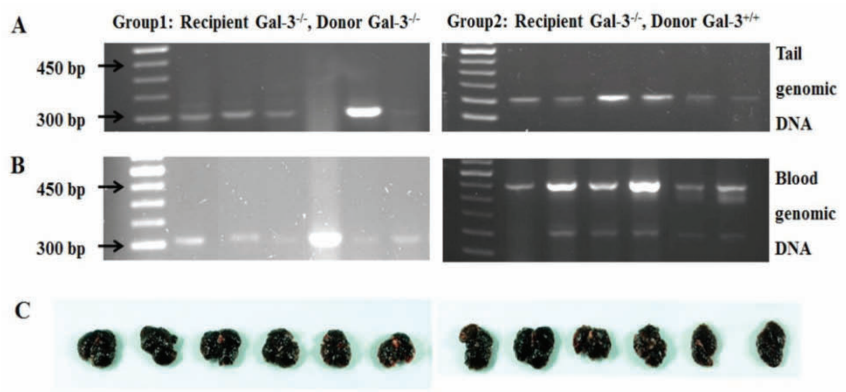


Fig.4.3.4. Experimental metastasis assay using bone marrow chimeric mice

In the this study, the importance of this interaction was proved by using modified citrus pectin which competed with lactose, and dominant negative inhibitor truncated galectin-3 which competed with endogenous galectin-3. To prove that polyLacNAc on tumor cells indeed brought about these effects via galectin-3; galectin-3 transgenic mice were used. Decreased metastasis of B16F10 cells correlated with galectin-3 expression on the lungs in galectin-3$^{+/+}$ and galectin-3$^{+/-}$ mice. However, galectin-3$^{-/-}$ mice showed a comparable colony number to galectin-3$^{+/+}$ mice. Surprisingly, reversal of metastasis in gal-3$^{-/-}$ mice suggested that host anti-tumor immunity might be compromised in these mice.

In order to investigate the role of galectin-3, mass spectrometric screen was performed in our lab to find galectin-3 binding proteins. It was found that, along with many other cell surface glycoproteins, CD147 was a major carrier of β1, 6 branched N-oligosaccharides. It was found to be localized in the cytoplasm after mutating all the glycosylation sites. The critical glycosylation sites required for membrane targeting of CD147 were identified.

Galectin-3 is a nucleo-cytoplasmic protein which is secreted out in a non-classical manner and often gets incorporated into the extracellular matrix component and basement membrane. The present study demonstrated that dynamics and organization of lamellipodial structures formed and signaling events for their formation on galectin-3 were very distinct as compared to those observed on very well studied extracellular matrix component such as fibronectin.

Our studies showed an upregulation of all survivin isoforms in oral cancer cell lines and tissues as well as predominant expression of ΔNp63 and secretory clusterin. Our studies also demonstrated that mutant p53 was capable of binding to p63 in vitro and affected the functions of p63. p63 activated survivin expression in the presence of the R273H mutant p53 whereas, in the absence of a functional p53, p63 repressed survivin expression. Similarly the tumorigenic properties regulated by p63 were also found to be affected by the presence of mutant p53. p63 knockdown showed reduced migration in irrespective of the p53 status of the cell lines. However, in the absence of a functional p53, p63 knockdown resulted in increased invasion whereas in the presence of a mutant p53 p63 knockdown resulted in decreased proliferative ability. Gene expression analysis identified genes involved in NOTCH signaling, Wnt signaling and TGFβ signaling to be under the regulation of p63 in oral cancer cells.

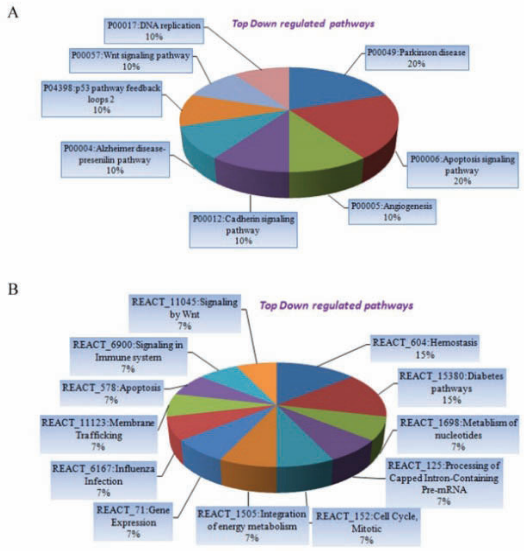


Fig. 4.3.5. Top downregulated PANTHER and REACTOME pathways in AW8507

Our studies thus demonstrated that p63 plays a role in oral tumorigenesis and also that the functions of p63 in oral cancer cells might be affected by the presence of the R273H mutant p53. This is the first study to show a gain of function role of the R273H mutant in oral cancers. Since oral cancers are frequently associated with mutations in p53, identification of the specific pathways activated by the mutant forms might provide a better approach to drug discovery and therapy.

Organelle size and shape inside a cell is a basic fundamental cell biological interest to study. Altered organelle size and shape is always associated with some clinical aspects. Karyoplasmic ratio (the ratio of the nuclear volume to cell volume) remains roughly constant in cells with widely different DNA contents, ranging from single-cell eukaryote to mammalian cells. It is tempting to speculate that there is a tight regulation of nuclear size and shape in normal cell and that regulation is disrupted in case of cancer cells. The current understanding of the size and shape control mechanism of the largest organelle nucleus is in its infancy.

In the present study, two model organisms were studied to understand nucleus size and shape control mechanism. The candidate clearly demonstrated alteration of both nucleus: cytoplasmic (N/C) ratio and size of nucleolus in different transformed cell lines compared to immortalized cell lines of the same tissue origin. The present concepts rely on nuclear size which is determined by a limiting soluble component that originates in the cytoplasm and is transported to the nucleus. If this is true, then nuclear import/export would be expected to play a role in determining nuclear size. In this study it was shown that perturbation of nucleo cytoplasmic transport could alter both N/C ratio and nucleolus size and number in immortalized cells. However, this increased N/C ratio could not further change the invasion potential of the same immortalized cells. Using an in vitro assay system, it was demonstrated that cytosolic factors controlled the size of the nucleolus. In mammalian system, communication between nucleus and cytoplasm is very important to maintain the N/C ratio and nucleolus size in immortalized cells. In the yeast system, using an unbiased approach, motor proteins (Kar3, Cin8) and pre mRNA splicing protein (Prp45) were found to control nuclear size and shape. In motor proteins Kar3, Cin8 and pre mRNA splicing protein Prp45 1-169, the nuclear shape was altered in all stages of cell cycle. This study indicated that prp45 is one of the important gene that controls nuclear shape as well as sub nuclear domain like chromatin unlike Kar3 and Cin8 null mutants. In yeast, nucleus size and shape alteration phenotype could be achieved through many different genes or pathways. Alteration in nuclear surface area or volume did not necessarily alter the chromatin inside the nucleus always.

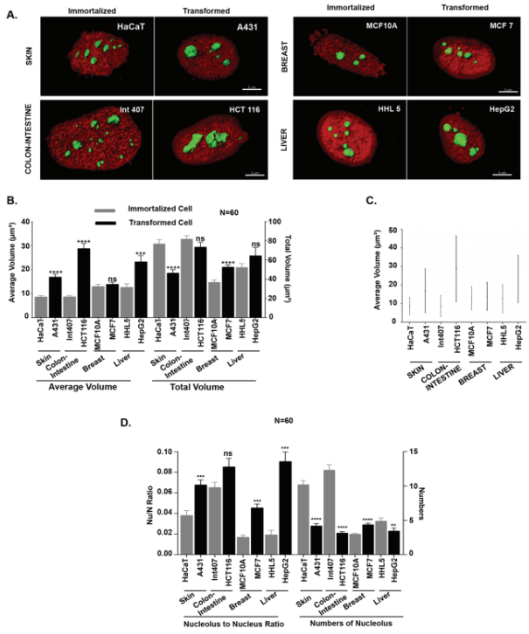


Fig. 4.3.5. Nucleolus size and number alters in transformed cell lines compared to immortalized counterpart

This very informative piece of work used both human cell lines and budding yeast to generate extremely interesting data that would be valued highly in the community for not only its novel insights but also for its systematic and measured approach.

Keratins are intermediate filament proteins predominantly expressed in epithelial cells. Keratins 8/18 (K8/18) pair forms a major intermediate filament network in simple epithelia. It is post translationally modified with phosphate and O-GlcNAc moiety at multiple serine residues. There are three *O*-GlcNAcylation (Ser29, Ser30, and Ser48) and two phosphorylation (Ser33 and Ser52) sites on K18, which are well characterized. Both these dynamic modifications have been reported to increase K18 solubility and regulate their filament organization. However, investigation of specific O-GlcNAcylation site responsible for regulation of functional properties of K18 has not yet been done. In this report, we investigated the site-specific interplay between O-GlcnAcylation and phosphorylation in regulating the functional properties of K18, like solubility, stability and filament organization. An immortalized hepatocyte cell line (HHL-17) stably expressing site-specific single, double, and triple *O*-GlcNAc and phosphomutants of K18 was used to identify the site(s) critical for regulating these functions. Keratin 18 mutation of *O*-GlcNAcylation at Ser30 (K18-S30A) exhibited reduced phosphorylation induced solubility, increased stability, defective filament architecture, and slower migration. Interestingly, K18-S30A mutants also showed loss of phosphorylation at Ser33, a modification known to regulate the solubility of K18. Further, the K18 phosphomutant (K18-S33A) mimicked K18-S30A in its stability, filament organization, and cell migration. These results indicated that *O*-GlcNAcylation at Ser30 promoted phosphorylation at Ser33 to regulate the functional properties of K18 and also impact cellular processes like migration. *O*-GlcNAcylation and phosphorylation on the same or adjacent sites on most proteins antagonized each other in regulating protein functions. Here we reported a novel, positive interplay between *O*-GlcNAcylation and phosphorylation at adjacent sites on K18 to regulate its fundamental properties.

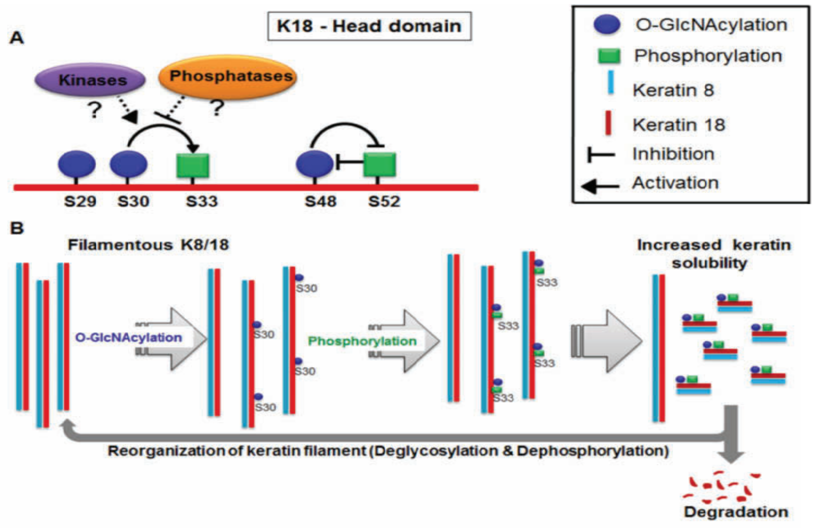


Fig. 4.3.6. Model depicting cross-talk between O-GlcNAcylation and phosphorylation at proximal sites on keratin 18 to regulate the solubility, degradation, and reorganization of the keratin filament network

Previous studies from our laboratory had demonstrated that antiapoptotic MCL-1 protein was overexpressed in human oral cancers and it contributed to acquired chemoradioresistance and poor prognosis. MCL-1 protein has a short half-life due to its rapid turnover by the ubiquitin-proteasomal degradation pathway. Although significant information is available regarding the genomic, transcriptional and posttranscriptional regulation of MCL-1, little is known about its posttranslational regulation. In the present study, we investigated the contribution of altered posttranslational regulation of MCL-1 protein, especially role of MCL-1-interacting proteins which modulate its degradation by the ubiquitin-proteasomal pathway, leading to its overexpression in oral cancers. We demonstrated that a deubiquitinase USP9X interacted with MCL-1 and mediated its deubiquitination, thereby enhancing its stabilization. The positive correlation between MCL-1 and USP9X expression was evident in oral cell lines as well as oral tissues. Moreover, targeted downregulation of USP9X led to a decrease in MCL-1 protein levels through its increased turnover. A small molecule WP1130-mediated inhibition of USP9X potently triggered apoptosis in oral cancer cells through downregulation of MCL-1 protein levels *in vitro* and *in vivo*. We also identified several novel MCL-1-interacting proteins by co-immunoprecipitation coupled with mass spectrometry; many of these belonged to the ubiquitin-proteasomal pathway. We also evaluated the efficacy of a BH3-mimetic small molecule anti-MCL-1 antagonist obatoclax against oral cell lines and demonstrated that it triggered a caspase-independent noncanonical cell death called “necroptosis” through induction of defective autophagy coupled with extensive mitochondrial stress. Our studies also showed a synergism between obatoclax and ionizing radiation and potent single agent *in vivo* efficacy of obatoclax. These studies underlined the potential of therapeutic targeting of MCL-1 and its prostabilizing mechanisms in human oral cancers.

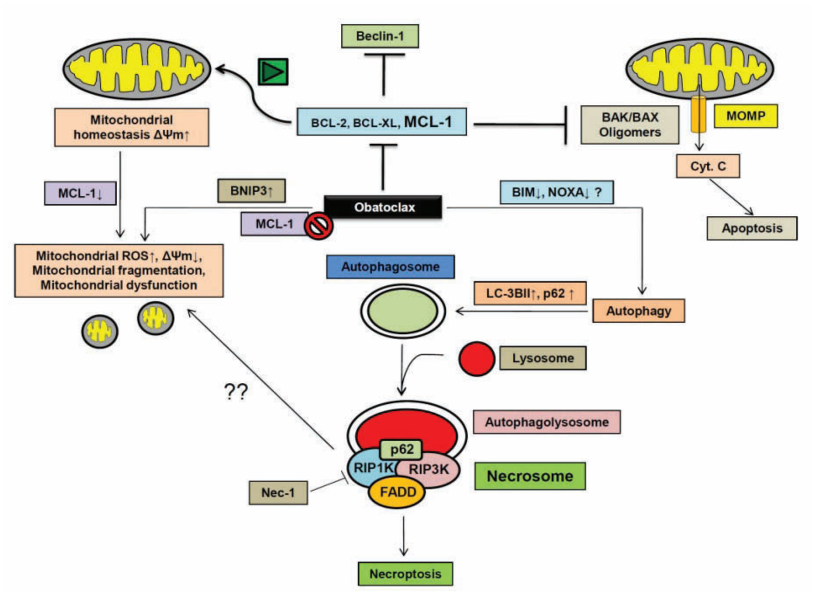


Fig. 4.3.7. The proposed mode of Obatoclax action in OSCC cells

Cancer Immunology

Involvement of galectin-3 in various steps of cancer progression and metastasis has been extensively documented. But, how endogenous galectin-3 expression levels in the host influence tumor growth and metastasis remains poorly understood till date. Further, the exact role of endogenous galectin-3 expression levels in the modulation of host anti-tumor immune responses and the mechanisms involved therein remain unclear and necessitate in-depth investigation.

In the present thesis, the role of endogenous galectin-3 in the regulation of host anti-tumor immunity and B16F10 lung metastasis was investigated using *LGALS3* transgenic mice, including Gal-3 wild type (Gal-$3^{+/+}$), Gal-3 hemizygous (Gal-$3^{+/-}$) and Gal-3 null (Gal-$3^{-/-}$) genotypic groups. Striking differences were observed in the immune scenario amongst these mice. Results indicated that absence of endogenous galectin-3 results in dysregulation of immune responses, reflected in increased T cell proliferation but reduced T cell Ca^{++} flux as well as ROS generation in stimulated splenocytes, decreased splenic NK cell frequency and NK cytotoxicity, marked decrease in serum Thl, Th2 and Th17 cytokine levels with disturbed serum cytokines milieu, reduced serum IFN-γ concentration, low frequency of IFN-γRl expressing splenic T and NK cells, and attenuation of STAT1 mediated IFN-γ signaling in Gal-$3^{-/-}$ mice under normal physiological conditions.

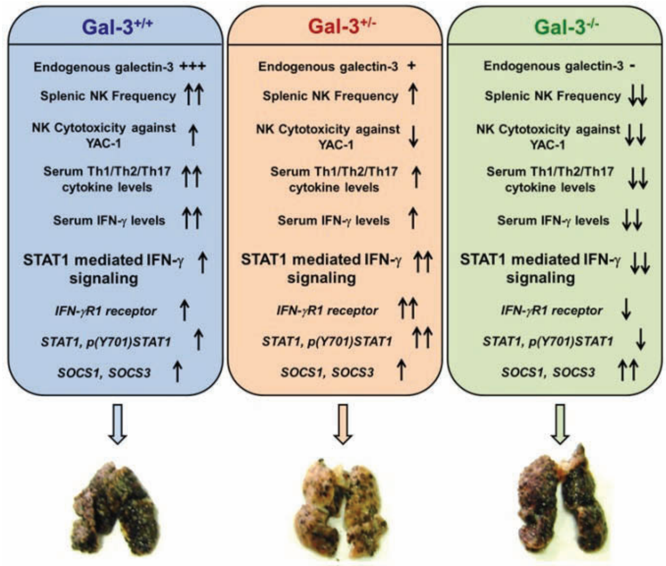


Fig.4.3.8. Role of endogenous gelectin-3 in anti-tumor immune responses

Experimental metastasis assay revealed that the ability of B16F10 murine melanoma cells to form lung metastatic colonies in Gal-$3^{+/+}$ and Gal-$3^{-/-}$ mice remained comparable and was significantly lower in Gal-$3^{+/-}$ mice. Under experimental metastasis assay conditions, Gal-$3^{-/-}$ mice splenocytes exhibited reduced NK cell frequency on day 14, higher proliferative responses, but reduced intracellular Ca^{++} flux and ROS generation upon *in vitro* stimulation. Further, the relative pattern of serum Th1, Th2 and Th17 cytokine concentrations in Gal-$3^{+/+}$, Gal-$3^{+/-}$ and Gal-$3^{-/-}$ mice changed gradually with progression of the lung metastasis. The enhanced B16F10 lung metastasis in Gal-$3^{-/-}$ mice could be strongly attributed to the compromised anti-tumor immunity observed in these mice.

Overall the results suggested that endogenous galectin-3 contributed to anti-tumor immune responses in the host. Endogenous galectin-3 expression levels in the host dictated the metastatic outcome through modulation of host immunity. The findings provided strong links to understand the crosstalk between galectin-3, immune system and cancer metastasis, which might facilitate the designing of more efficient galectin-3 targeted therapeutic strategies against cancer in the future.

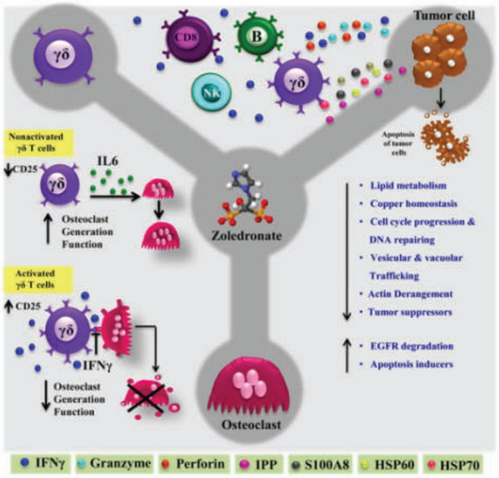


Fig.4.3.9. Crosstalk between bone and γδ T cells in breast cancer patients mediated by Zoledronate

Aminobisphosphonates are given as a standard treatment modality to patients with osteoporosis or with skeletal malignancies associated with breast cancer or multiple myeloma. The present thesis investigated the crosstalk and mechanism of action of aminobisphosphonate (Zoledronate) on breast tumor cells, immune cells (γδ T cells) and osteoclasts. The work embodied in the thesis demonstrated that activation status of the γδ T cells and cytokine dynamics (IFNγ/ IL6) dictated their anti or pro osteoclastogenic behavior. A proteomic approach using MALDI/TOF-TOF and LC-MS identified unique proteins and cellular pathways that were treatment with Zoledronate. Zoledronate created a 'metabolic crisis' in the breast tumor cells and induced apoptosis. The data obtained also identified molecules (IPP, HSPs and S100A8) that played an important role in γδ T cell mediated recognition of Zoledronate treated tumor cells. In the translational

component of the thesis, immune profiles of the healthy individuals, treatment naïve breast cancer patients and Zoledronate treated breast cancer patients [who were exhibiting bone metastasis] were generated. Investigation of immune cell subsets, cytokine profiles, activation markers, memory markers and effector molecules on γδ T cells / αβ T cells was carried out using multicolor flow cytometry. The study demonstrated increased percentages of activated γδ T cells, majorly of terminally differentiated effector memory RA$^+$ type (TEMRA, highly cytotoxic), showing increased expression of CD25 and IFNγ in Zoledronate treated breast cancer patients. γδ T cells isolated from Zoledronate treated breast cancer patients also showed reduced IL6 secretion (pro-osteoclastogenic and pro-tumorigenic cytokine). The present study demonstrated that Zoledronate facilitated tripartite crosstalk between tumor cells, immune cells and bone cells and also highlighted the effect of Zoledronate in breast cancer patients, which was significantly different from its well defined anti-resorptive function.

Oral cancer is the third most common cancer in India due to the high prevalence of tobacco chewing, smoking and alcohol consumption. Immune dysfunction appears to be more frequent and profound in cancer patients because of the accumulation of immunosuppressive factors /cells in the tumor microenvironment. The focus of the study was to identify factors secreted by oral tumors that affect the key T signaling events and to address the crosstalk of immunosuppressive cells such as myeloid-derived suppressor cells and regulatory T cells in inhibiting the antitumor immunity in oral squamous cell carcinoma (OSCC) patients.

This study unravelled different regulators which have the competency to dampen the antitumor immune response in oral cancer patients. For the first time, a potentially important function of tumor-derived OAS2 as a paracrine negative regulator of T-cell functions was identified. The mechanism employed by TNF-α, an important negative regulator of T cell function was also addressed. Blocking TNFR2 enhanced the TNF-α induced T cell dysfunction suggesting that use of antagonist ligands aimed at a single receptor, TNFR2 holds the potential for selectively turning off immunosuppressive microenvironment. However, at the same time, it might lead to TNF-α induced TCR signaling defect in antigen encountered T cells via TNFR1.

Notch signaling was found to be one of the positive regulators of T cell signaling; inhibition of this signaling was seen to affect proximal as well as distal signaling molecules. The study provided insights into mechanisms that integrated TCR and cytokine signals to determine the outcome of T cell response and identified a central role for notch signaling in this process. Our data highlighted novel molecular targets for the manipulation of T-cell dependent immunity with important implications for cancer immunotherapy.

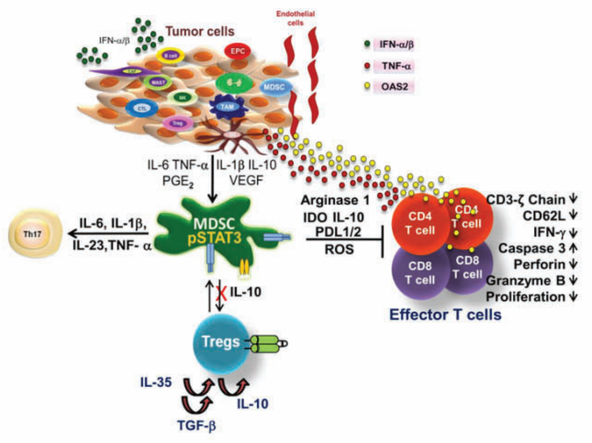


Fig. 4.3.10. Immunosuppressive network in oral cancer patients

Tumor microenvironment is characterized by chronic inflammation and accumulation of immune suppressive cells like myeloid derived suppressor cells (MDSCs) and regulatory T cells (Tregs). These cells are responsible for suppression of T cell activation and dampening anti-tumor immunity. MDSCs were elevated in human OSCC patients, indicating that they contributed to immune suppression and their levels correlated with cancer stage. STAT3 played an important role in MDSC activation and accumulation in OSCC patients. OSCC patients had elevated Tregs and correlated with IL-10 produced by MDSCs. However, MDSCs did not induce Treg generation under *in vitro* conditions. MDSCs induced TH17 generation and IL17 producing cells were higher in OSCC patients. This suggested that MDSCs contributed in enhancing the inflammation as well as inducing T cell tolerance in oral cancer patients. Understanding the mechanism of action of immune suppressive cell populations in OSCC patients is important in designing effective immunotherapeutic modality.

Gall bladder cancer (GBC) is a relatively uncommon but lethal biliary tract related cancer with 5 year survival less than 5%. Complete surgical resection is the only curative option available, but more than 90% GBC patients are with un-resectable disease. Despite improved results of chemotherapy and surgery, the long term outcome remains disappointing. Around 70-80% patients are associated with chronic inflammatory condition of cholelithiasis.

The present prospective study aimed at investigating the role of inflammatory immune infiltrates contributing to GBC. Immunophenotyping in GBC patients revealed that the cells contributing to adaptive immunity ($CD3^+$, $CD4^+$, $CD8^+$ T cells) were decreased in peripheral blood of GBC patients compared to healthy individuals (HI).

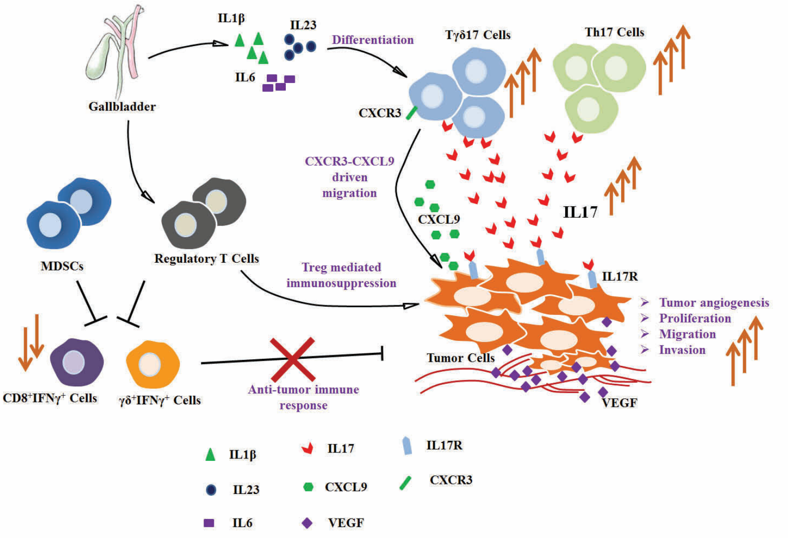


Fig. 4.3.11. Role of pro-inflammatory (T γδ17, Th 17 and Tc17) cells and immunosuppressive Regulatory T cells (Treg) in progression of Gall Bladder Cancer

Downregulated expression of CD3-ξ chain in T cells, low lymphocyte proliferative response and decreased secretion of effector cytokines upon stimulation with anti-CD3 mAb and mitogen suggested that the immune response in GBC patients was dysfunctional.

Investigation of inflammatory immune cells revealed that the levels of IL17 producing subtype of $\gamma\delta$-TCR^+ (Tγδ17), $CD4^+$ (Th17) and $CD8^+$ (Tc17) T cells were increased in peripheral blood (PBL) and tumor infiltrating lymphocytes (TIL) of GBC patients compared to HI. Data demonstrated that Tγδ17 cells specifically secreted

IL17 and elicited production of VEGF and other angiogenesis related factors in gallbladder tumor cells. Tγδ17 also induced vascularization of chorioallantoic membrane through IL17. Addition of recombinant IL17 to gallbladder tumor cells (OCUG1 cell line) induced proliferation, migration, matrigel invasion and VEGF production in a concentration dependent manner. For the first time it was shown that Tγδ17 cells migrate towards gallbladder tumor using CXCR3/CXCL9 chemokine axis. The cytokines required for differentiation and/or stabilization of Tγδ17 cells (IL6, IL23, IL1β) were elevated in the sera as well as in the tumor environment of GBC patients. Analysis of CD4$^+$CD25$^+$CD127$^{low/-}$ regulatory T cells revealed that the levels of Tregs were decreased in PBL but their suppressive potential was not compromised. Study of dynamics of these cells revealed that in TILs, the ratios of Th17/Treg, Tγδ17/Treg and Tc17/Treg increased but CD8$^+$IFNγ$^+$ and γδ$^+$IFNγ$^+$ cells were decreased. Moreover, Tγδ17, Th17 and Tc17 cells were elevated in GBC patients irrespective of clinical stage of patients. Survival analysis showed that Tγδ17, Th17 and Treg cells in peripheral blood were associated with poor survival of GBC patients.

Taken together, our data strongly suggested that Tγδ17 is a pro-tumorigenic subtype of γδT cells and was emerging as a “druggable immune target” that played an important role in GBC progression. Thus, future immunotherapeutic treatment strategies for GBC might use a combined approach to block the trafficking of Tγδ17 cells to the tumor and inhibit the functions of IL17.

An earlier study from our lab on Indian T-ALL patients had identified clonal TCR γ and δ junctional gene rearrangement status of T-ALL as a potential prognostic marker. Clinically, survival probability was found to be significantly higher in TCRγδ+ as compared to TCRαβ+T-ALL patients when γ and δ gene rearrangement was considered as prognostic variable. This observation provided an impetus to investigate how TCRγδ+T-ALL differed biologically from TCRαβ+T-ALL subgroup. The present study identified TCRγδ+T-ALL as a distinct subgroup from TCRαβ+T-ALL using gene expression profiling. TCRγδ+T-ALL subgroup with wild type/heterozygous copies of CDKN2A/B showed significantly (p=0.017 and p=0.045, respectively) improved DFS as compared to TCRαβ+T-ALL. This study for the first time identified CDKN2A/CDKN2B copy number variations combined with TCR clonality as a potential prognostic marker in T-ALL patients. The differences in the two subgroups of T-ALL patients were studied further at the functional level. TCR γδ clonal leukemic blasts showed significantly better immune synapse formation with γδ T cells over TCR αβ clonal leukemic blasts. TCRγδ+T-ALL patients showed higher expression of γδ T cell subsets, perforin molecules, CM and TemRA cells, NKG2D receptor, and activation markers. Differences in the effector immune cell composition and efficient immune synapse formation of TCR γδ clonal blasts explained the survival advantage of TCRγδ+T-ALL patients. The study also analysed the immune scenario

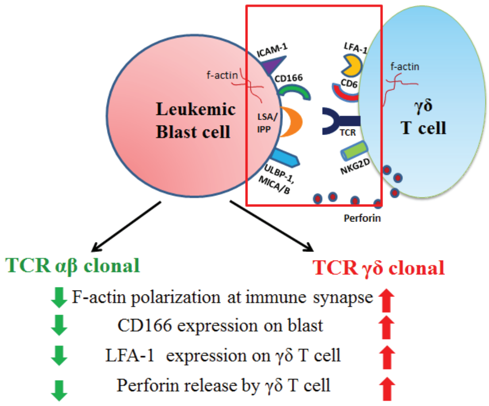


Fig. 4.3.12. TCRγδ+T-ALL is a distinct subgroup from TCRαβ+T-ALL

in T-ALL patients at diagnosis and remission, and compared these profiles with healthy individuals. T-ALL patients at diagnosis showed significant low numbers of CD3+, T helper, T cytotoxic, αβ T, γδ T, NK and NKT cells. γδ T cells played an important role in remission patients, as the number of activated γδ T cells and the expression of perforin molecules in γδ T cells was increased compared to patients at diagnosis. The role of γδ T cells in ALL patients undergoing allogeneic BMT was also studied. It was observed that recipients showed significantly less CMV reactivation if donors had high γδ T cells. It was observed that donor's immune cell composition affected the clinical outcome of recipients, and could be used as a predictor of disease outcome. In conclusion, γδ T cells could be used as prognostic indicator and promising immunotherapeutic modality in T-ALL patients.

Cancer Genomics

Medulloblastoma is classified in four distinct molecular subgroups, viz. WNT, SHH, group 3 and group 4. These subgroups also differ in their microRNA profile, with the WNT subgroup tumors having the most distinctive microRNA profile with a number of microRNA upregulated in the WNT subgroup as compared to other subgroups as well as the normal cerebellum. The present study was undertaken in order to understand whether transcription of WNT subgroup specific miRNAs viz. miR-193a, miR-148a, miR-365 and miR-224 was directly or indirectly regulated by WNT signaling pathway. Further the role of miR-148a in modulating proliferative, migratory and tumorigenic potential of medulloblastoma cells was also investigated. Activity of both miR-148a and miR-193a promoter was found to be induced upon expression of MYC, a known target of the WNT signaling pathway. Bisulfite sequencing of MiR-148a promoter region showed hypermethylation of CpG island in non-WNT medulloblastoms and in established group 3 medulloblastoma cell lines. Treatment with HDAC inhibitor brought about upregulation of miR-148a expression in a medulloblastoma cell line. Thus, MiR-148a expression in WNT subgroup medulloblastomas appeared to be induced by MYC expression while its expression was suppressed in non-WNT medulloblastomas as a result of epigenetic modifications.

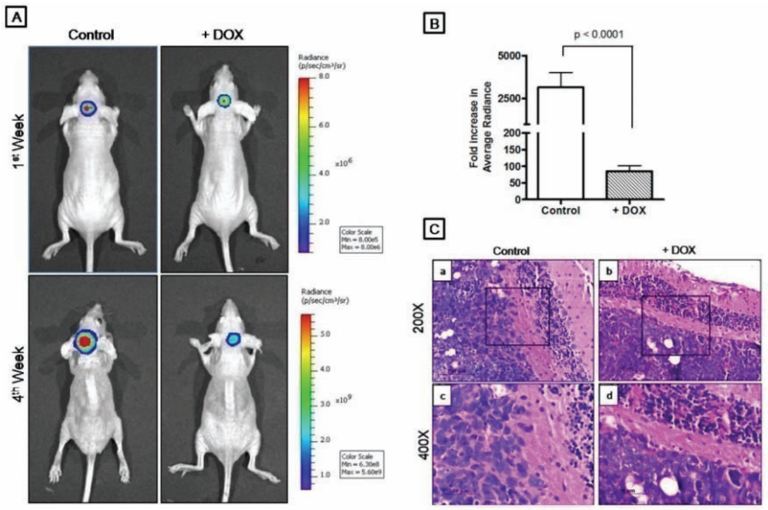


Fig. 4.3.13. Effect of miR-148a expression on tumourigenic potential and in vivo invasion potential of D283 cells studied by intracranial xenograft mouse model

MiR-148a was expressed in non-WNT medulloblastoma cell lines at levels comparable to that in the WNT tumors using inducible lentiviral vectors. MiR-148a expression was found to inhibit growth and brought about reduction in the clonogenic potential, invasion potential and tumorigenicity of medulloblastoma cells. Neuropilin 1 was identified as a novel miR- 148a target gene in medulloblastoma. MiR-148a mediated inhibition in invasion potential and *in vivo* tumorigenicity of medulloblastoma cells was restored upon NRP1 expression, indicating the importance of NRP1 as a key miR-148a target gene in medulloblastoma. Furthermore, NRP1 expression in medulloblastomas was associated with poor survival, with little or no expression in the majority of the WNT tumors, indicating its usefulness as marker for prognostication. The tumor suppressive effect of miR-148a expression accompanied by the down-regulation of NRP1 makes miR-148a an attractive therapeutic agent for the treatment of medullo blastomas.

Cancer research has seen unprecedented progress in the past decade with identification of various molecular alterations driving tumor growth leading to specific therapeutic solutions targeting these molecular alterations. To adopt such treatment options for the Indian population, in-depth characterization of tumors among Indian patients remains a paramount requirement. This study provided solutions for three most predominant cancer types prevalent in India -- lung cancer, head & neck cancer and cervical cancer. It identified a novel therapeutic target in lung adenocarcinoma, established rare patient derived cell lines as representative models of several known and novel genomic alterations of head & neck cancer, and provided a landscape of HPV infection in cervical cancer along with open source computational tool HPVDetector for the effective utilization of NGS platforms for HPV analysis by a wider community. The first landscape of therapeutically relevant alterations in lung adenocarcinoma of Indian origin, using advanced sequencing and mass-spectrometry technologies across 363 patient samples was presented. This study led to the discovery of novel recurrent mutations in fibroblast growth factor receptor 3 (*FGFR3*) gene, which were validated to be oncogenic and sensitive to pharmacological inhibition using *in-vitro* and *in-vivo* approaches. A proof-of-principle strategy for deriving biological interpretation from studies

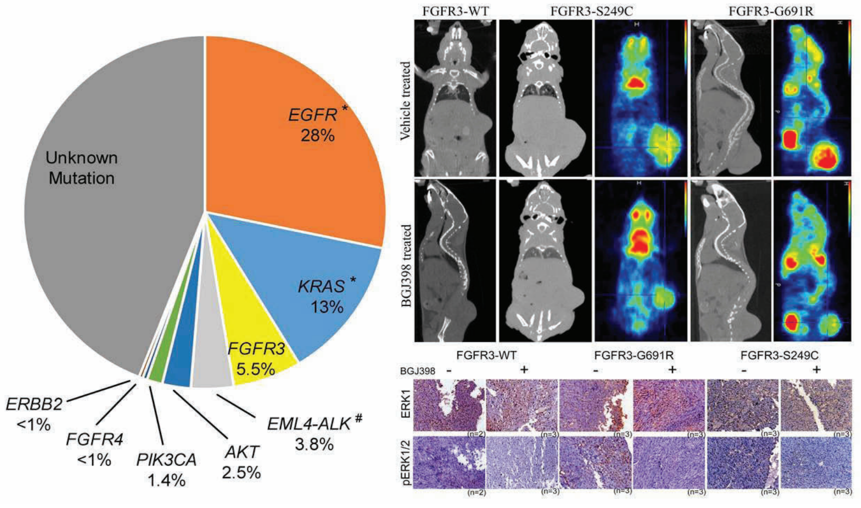


Fig. 4.3.14. Drug-sensitive FGFR3 mutations in lung adenocarcinoma

involving fewer samples by performing integrated genomics analysis was presented. In brief, four rare cancer cell lines derived from head & neck cancer patients of Indian origin were characterized by adopting a posterior filtering approach. This allowed us to identify most of the major hallmark alterations in head & neck cancer, otherwise possible to be determined only using larger sample cohort. In addition, the study also led to the discovery of a novel oncogene nuclear receptor binding protein (*NRBP1*) gene in head and neck cancer. A user-friendly open-source computational tool “HPVDetector” for non-computational researchers was developed to help them analyze the next-generation sequencing datasets to detect the traces of human papillomavirus (HPV). The tool is easy to install, has minimal third party dependencies and comes along with graphical user interface (GUI).

We presented an integrative genome-wide analysis of copy number alterations (CNAs) and gene expression changes in HPV negative, gingivobuccal complex (GBC) pre-cancerous lesions (leukoplakia) and oral squamous cell carcinoma (OSCC) patients. We could identify CNAs and differentially expressed transcripts that could be used to predict the risk of progression from leukoplakia to OSCC. The genomic profiles of leukoplakia resembled those observed in the later stages of OSCC; several changes were associated with this progression, including amplification of 8q24.3, deletion of 8p23.2, and dysregulation of *DERL3, EIF5A2, ECT2, HOXC9, HOXC13, KRT76, MAL, MFAP5* and *NELL2*. Furthermore, we demonstrated for the first time that *KRT76* loss is one of the early events, but not essential for cell transformation. Comparing copy number profiles of primary tumors with and without lymph node metastasis, we identified alterations associated with nodal metastasis, including amplifications of 3p26.3, 8q24.21, 11q22.1 and 11q22.3 and deletion of 8p23.2. Additional analysis demonstrated up regulation of *BIRC2* (cIAP1) and *BIRC3* (cIAP2) in tumor samples with lymph node metastasis and, based on functional validation, we could identify role of cIAP2 (*BIRC3*) in lymph node metastasis in SCC29B cells. Integrative analysis revealed several biomarkers that had never or rarely been reported in previous OSCC studies, including amplifications of 1p36.33 (attributable to *MXRA8*), 3q26.31 (*EIF5A2*), 9p24.1 (*CD274*), and 12q13.2 (*HOXC9* and *HOXC13*). Additionally, we found that amplifications of 1p36.33 and 11q22.1 were strongly correlated with a poor clinical outcome. Overall, our findings delineated genomic changes that could be used in treatment management for patients with potentially malignant leukoplakia and OSCC patients with higher risk of lymph node metastasis.

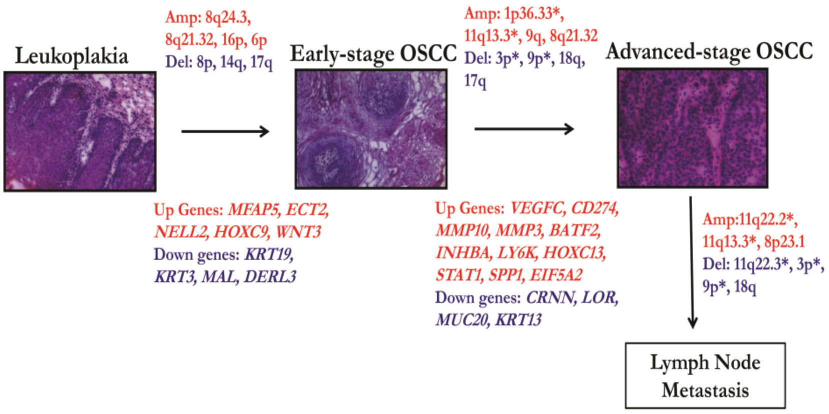


Fig.4.3.15. Summary of the predictive genomic and transcriptomic signatures associated with gingivobuccal cancer progression from pre-invasive lesions (leukoplakia) to cancer and lymph node metastasis. (*) represents alterations associated with disease specific survival in OSCC patients

Raman Spectroscopy

Oral cancer is the 16th most common cancer in the world and the most common malignancy in Indian men. The survival rates for oral cancer have not improved in several decades. Delays in diagnosis and recurrences are the major causes for the low survival rates. Visual inspection followed by biopsy and histopathological examination is the gold standard for oral cancer diagnosis; however these approaches have associated limitations. As early diagnosis can improve survival rates and overall patient outcomes, there is a need to develop rapid, objective and patient friendly less-invasive/ non- invasive approaches for screening and early diagnosis. Raman spectroscopy (RS), a vibrational spectroscopic approach based on inelastic scattering of light, has shown promise in cancer diagnosis. In the present study, the potential of RS in early oral cancer diagnosis and sub-site classification was explored using both ex vivo (serum and exfoliated cells) and in vivo approaches. Serum RS was explored for oral cancer diagnosis and sub-site classification using both resonance (n=70) and conventional Raman (n=86) studies. Similar classification was observed for normal and oral cancer groups; even buccal mucosa and tongue cancers could be classified. Further, the potential of serum RS in screening was observed using 339 samples where normal could be distinguished from other disease conditions (premalignant, disease control and oral cancer) with sensitivity and specificity values comparable to existing screening approaches like Pap and mammography. Exfoliated cells collected from healthy without tobacco (n=40), healthy with tobacco (n=40), oral premalignant (n=27) and malignant subjects (n=31) were subjected to Raman spectra acquisition and Pap staining (for cytological correlation).

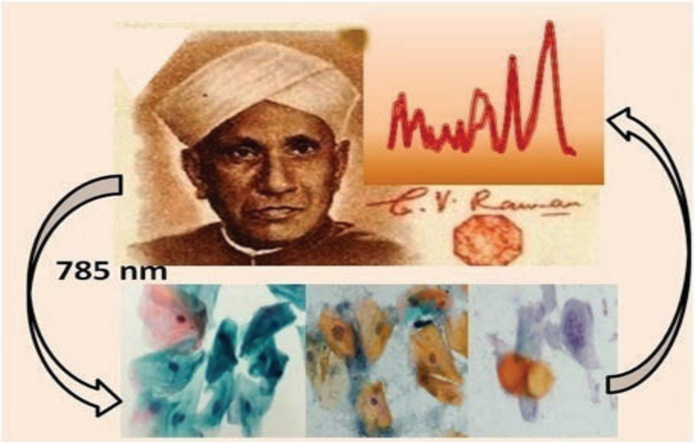


Fig. 4.3.16. Raman exfoliated cytology

These samples were analyzed in two different studies; *proof-of-concept* where differences between healthy and oral cancer were explored and *early diagnosis* where feasibility to detect premalignant cells was evaluated. Healthy could be successfully differentiated from tumor cells; lower classification was observed in premalignant samples. In vivo studies were undertaken as a non-invasive modality to diagnose cancer at different subsites: buccal mucosa, lip and tongue using healthy (n=72) and oral cancer subjects (n=85). In the first step, anatomical differences between these three subsites were evaluated in healthy, contralateral, premalignant and malignant conditions. Subsequently, diagnostic algorithms to distinguish healthy, contralateral, premalignant and malignant conditions were built for individual and then pooled subsites. The pooled subsites approach was found to be more meaningful for screening applications. Thus, the findings of this thesis demonstrated the potential of RS in oral cancer diagnosis and screening using both less-invasive and non-invasive approaches. Large-scale clinical and field trials are necessary before prospective clinical translation can be realized.

Oral cancers are a major health concern in South Asian nations. Despite advancements in treatment modalities, oral cancers still suffer from a poor 5-year survival rate (~50%), attributable to late detection. Thus, early detection is required for successful management of oral cancers. Currently practiced diagnostic gold-standard, biopsy followed by histopathology, is invasive (and painful), prone to subjective errors and not convenient for repeated sampling. Hence, Raman spectroscopy (RS) - a rapid, objective, non-invasive technique, sensitive to tissue biochemistry, could be effective in early diagnosis, as biochemical changes precede visible morphological alterations during carcinogenesis. RS has shown promising results in diagnosis of several cancers. Such in vivo studies have mostly relied on clinical examination for site of spectral acquisition. Hence, the present study was undertaken on the widely used hamster buccal pouch (HBP) model for RS based investigation of sequential progression of oral carcinogenesis, verified vis-a-vis histopathology.

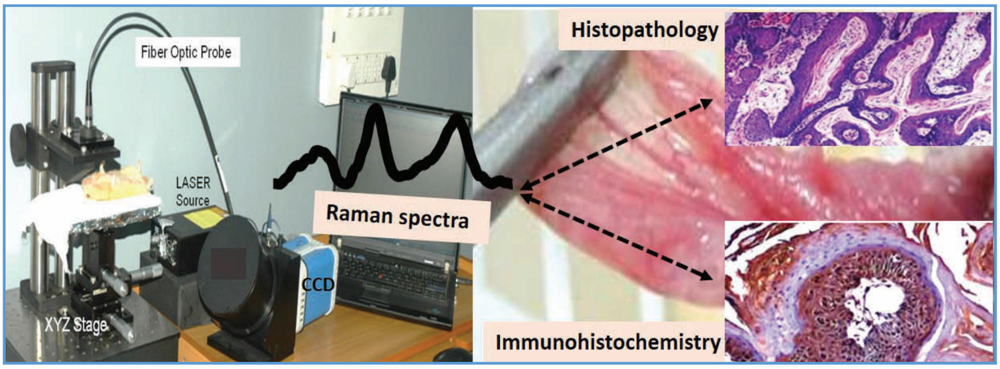


Fig.4.3.17. Raman spectroscopy in experimental oral carcinogenesis

In the first objective, week-wise analysis was carried out using both in vivo and ex vivo approaches. Sensitivity was 70% by week 8, 70-80% by week 9 to 11 and 80-100% by week 12 to 14. Thus classification increased progressively till 8 weeks, reached a plateau phase between 8 and 12 weeks and finally increased up to 100% by 14 weeks. In the second objective, spectral models were trained using histopathology and biomarker expression. Results showed increasing incidence of higher pathologies (dysplasia/ SCC/ G2, G3) with progression of weeks (3% for week 1-3 to 89% for week 12-14). Misclassifications were explored further and it was shown that repeated mechanical irritations might also lead to abnormal changes in tissues. These changes revealed small foci of higher pathologies and also higher expression of cyclin D1 with respect to normal regions. Overall, the findings suggested potential of RS in monitoring progression during carcinogenesis in buccal pouch, and in identifying abnormal changes and microheterogenity which might often go unnoticed in clinical examinations and conventional studies wherein tissue extracts/homogenates are employed. Results provided further proof of RS being a potential adjunct for prospective non-invasive, label-free screening in the general population, vis a vis conventional screening which was shown to be effective in high risk groups.

DNA Repair

In this study, we addressed the fundamental issue of radiation resistance in Glioblastoma Multiforme (GBM) a highly malignant form of brain tumor. However, because of inaccessibility to the inherently resistant cells responsible for recurrence in GBM, our understanding of the survival strategies adopted by the tumor cells has been limited. To circumvent this problem, we recapitulated clinical scenario of GBM resistance in a cellular model developed from fresh naïve primary GBM patient samples and cell lines. Using our model, we showed that upon lethal dose of radiation, a small percentage of GBM cells survived, were non-apoptotic and transiently became non- proliferative. They were arrested in G2/M phase of cell cycle mediated by inhibitory phosphorylation of Cdk1(Y15) and p21. Surprisingly we found that although these radiation resistant cells (RR) were non -proliferative, they were highly motile and underwemt homotypic cell-cell fusion at a high frequency to form multinucleated and giant cells (MNGCs). Cell fusion led to the induction of senescence as seen by β-galactosidase staining; high expression of SASPs (senescence associated secretory proteins) was also observed. SASPs provided survival and proliferation signals to the cells in an autocrine manner and thus allowed RR cells to regrow and give rise to

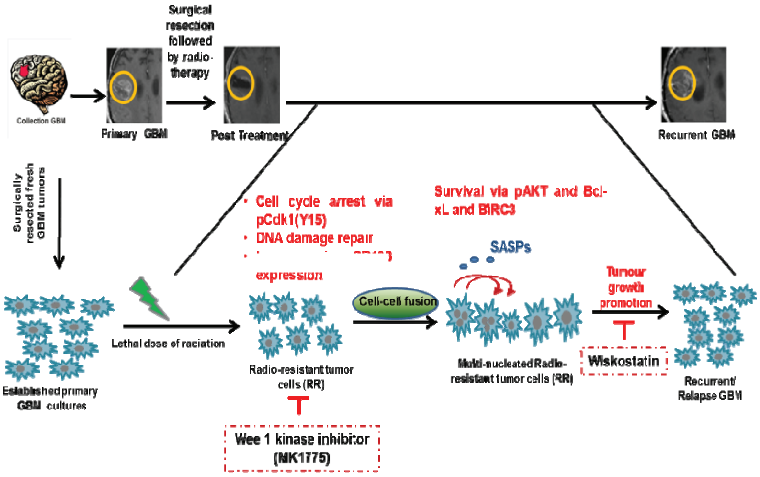


Fig.4.3.18. Recapitulating clinical scenario of GBM resistance in a cellular model

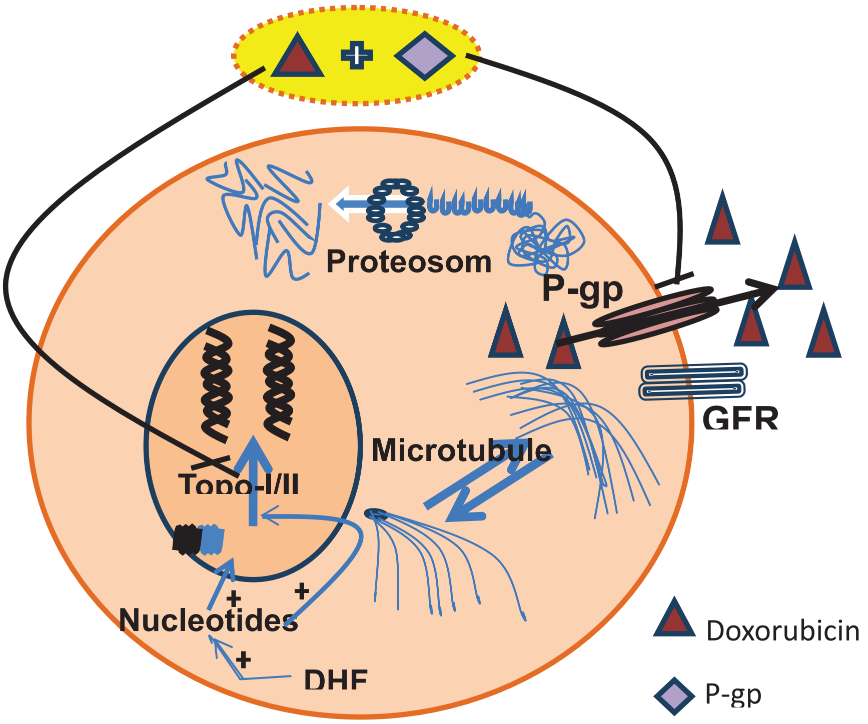
recurrent cells. We also found enhanced expression of anti-apoptotic genes BIRC3 and Bcl-xL mRNA as well as active AKT in RR cells which synergistically regulated apoptosis. Importantly, we showed that the duration of the resistant cell formation was associated with poor prognosis in GBM. Since DNA damage repair (DDR) pathway plays a significant role in maintaining genomic stability, we wanted to understand how MNGCs modulated their DDR pathway. We showed that MNGCs activated ATM-Chk2 or ATR-Chk1-RPA2 axis, repairing their DNA by non homologous end joining (NHEJ) pathway and not by homologous recombination. Given the association of DDR and histone methylations, we found up-regulation of H3K36me2 and SETMAR methyltransferase predominantly in the RR cells displaying euchromatin architecture. H3K36me2 is known to enhance recruitment of NHEJ repair components including Ku80. Accordingly, we demonstrated that mutating H3.3 at lysine 36 or knockdown of SETMAR in RR cells decreased the NHEJ repair response at the DSB site and alleviated survival of resistant cells. Additionally, inhibition of NHEJ pathway using DNA-Pk inhibitor NU7026 decreased the survival capacity of radiation resistant cells.

In summary, our data provided a mechanistic explanation and novel insights into an unexplored multi-step process of radiation survival and recurrence in Glioblastoma. We identified novel homotypic cell fusions of resistant glioma cells which modulated histone methylation, promoting NHEJ-driven repair of DSBs. These novel mechanisms facilitated survival and recurrence, thereby generating a rationale for developing combinatorial therapies.

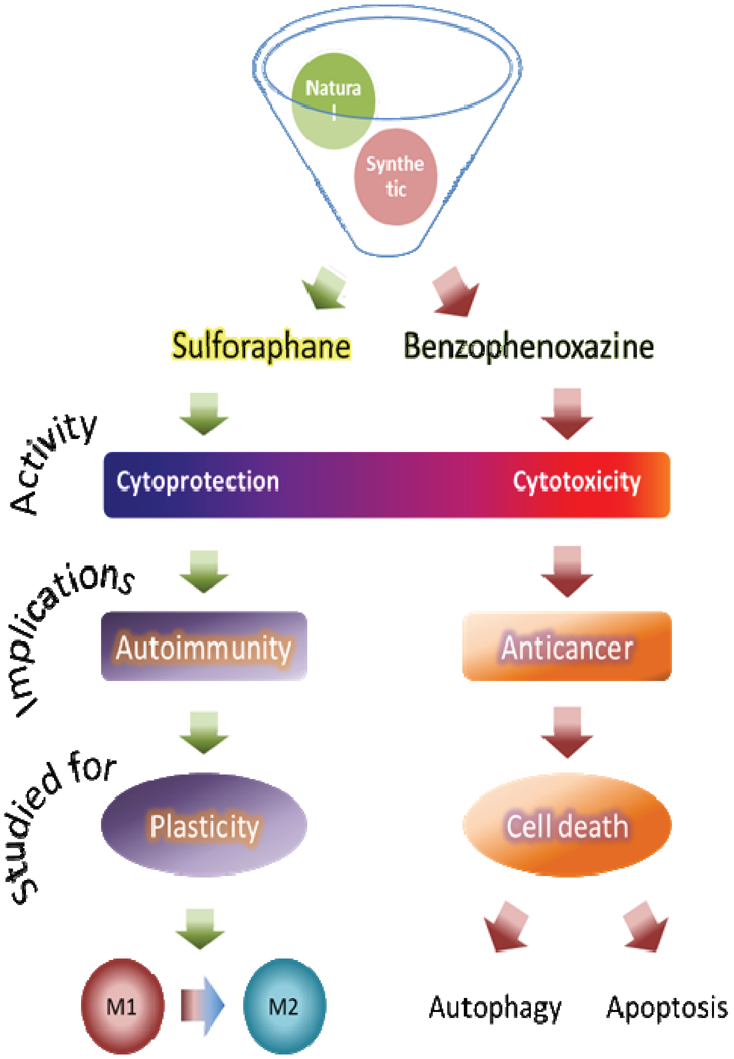
4.4 National Institute for Science Education and Research (NISER), Bhubaneswar

During the period, 5 students were awarded Ph.D. degree in Life Sciences. Highlights from some the theses are presented as follows.

Acquired drug resistance is a leading cause of treatment failure and relapse as significant resistant cells are left unaffected. P-glycoprotein (p=gp) is considered being a prime mechanism for drug resistance. The present work is based on the hypothesis to develop nanoformulations for circumvention of chemo-resistance in a cancer model system. Here, different combinational nano-formulations (liposomes, micelles and liposomes) containing doxorubicin with p-gp inhibitors (curcumin and biochanin-A) were developed, characterized and studied for reversal of chemoresistance.

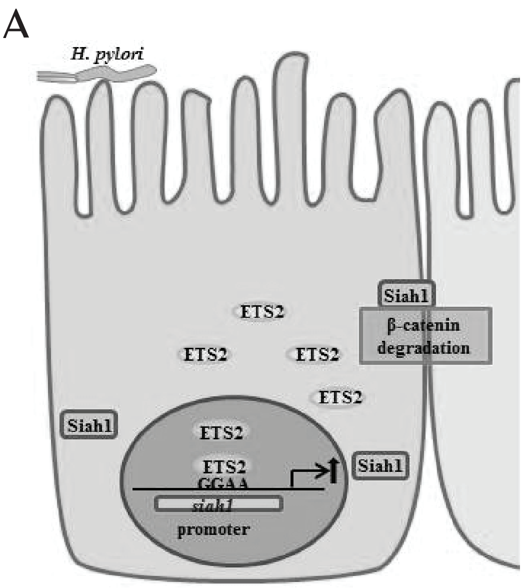


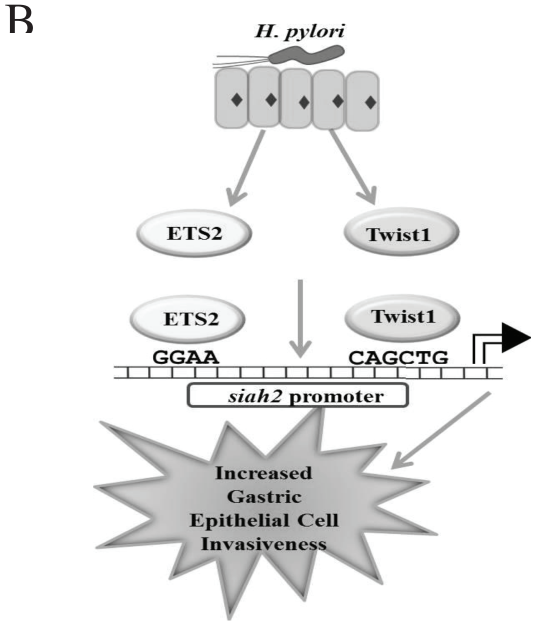
Understanding the outcome of a cellular response for a given ligand is an important pre-requisite to foster the implication of any chemico-biological interaction in drug research. In the current work, a hormetic phytochemical sulforaphane (SFN), popularly known as an anticancer agent was studied for its autoimmune response in non-cytotoxic doses. From the thesis work it was demonstrated that in a collagen-induced cell based autoimmune model, SFN induced phenotypic plasticity shifting the balance of anti-inflammatory M1 macropahges more towards anti-inflammatory M2. In another study, three derivatives of benzophenoxazine compounds were studied for mode of cell death in chemorefractory COLO205 (colon cancer) and apoptosis-resistant MiaPaCa2 (pancreatic cancer) cell line. Detailed study show that the compounds were able to trigger apoptotic cell death in the chemorefractory BRAF V600E COLO205 cells while in the apoptotis-resistant MiaPaCa-2 cells it induced autophagy. Further validations and more derivatives from this chemical class are underway.



Work focused on an alternative paradigm to test if (a) efficacy of immune stimulants such as Host Defense Peptides (HDP) can be significantly enhanced by conjugating with nanoparticles and nanotubes and (b) established comparative efficacies of potential probiotics that are widely prescribed for supplementary therapy. Work showed that upon conjugation of Indolicidin and LL-37 with carbon nanotubes and gold nano-particles, efficacies of these HDPs can be enhanced by 1000-fold and also established the major mechanistic pathways of action in vitro. Work further established that *Lactobacillus acidophilus* (LA) can effectively clear Salmonella infection and enrich short-chain fatty acid metabolised gut microbes in Th2 biased mice over Th1-biased mice.

Metastasis is a multistep process involving epithelial-mesenchymal transition (EMT). Cancer cells that become metastatic in nature are more treatment-resistant and targeted killing of these cells are hard to achieve. This thesis work explored how hypoxia and *Helicobacter pylori* regulated gastric cancer EMT and metastasis. Both of these factors upregulated hypoxia-inducible factor 1α (Hif1α), which required p300 as a transcriptional coactivator. This role of p300 depended largely on histone acetyltransferase (HAT) activity. Suppression of HAT by CTK7A downregulated metastasis and induced Noxa-mediated apoptosis selectively in *H. pylori*-infected and hypoxic gastric epithelial cells.





Siah proteins are E3 ubiquitin-ligases which are important in several fundamental cellular processes. So far, Siah1 was known to be apoptotic while Siah2 was known as a tumor-promoter. This thesis work identified that *Helicobacter pylori* induced expression of the transcription factor ETS2 which enhanced Siah1 expression in gastric cancer cells (GCCs) while Siah2 expression in *H. pylori*-infected GCCs was induced by ETS2 and Twist1. *H. pylori*-infected GCCs showed more invasiveness after overexpression of *siah1* and *siah2* genes. Proteasomal degradation of cell membrane-bound β-catenin by Siah1 promoted gastric cancer metastasis while Siah2 showed nuclear accumulation in *H. pylori*-infected GCCs in the Figures A and B.

5. Mathematics

During this period, HBNI awarded Ph.D. degree to 19 students who carried out research in Mathematics at different CI/OCC of HBNI. Highlights of research specific to different CI/OCC are as follows.

5.1 Harish-Chandra Research Institute (HRI), Allahabad

During the period, 7 students were awarded Ph.D. degree in Mathematics. Highlights from some the theses are presented as follows.

The first two chapters of one thesis deal with the results related to Riesz sum and last chapter comprises of results concerning k-free integers. The first chapter is based on a result related to Riesz Sum. In a joint work with Jay Mehta, we have given another proof of well-known Wilton's formula to obtain the linearized product of two Riemann zeta functions. In the second chapter, a brief review of Dirichlet divisor problem starting with its definition, history and present development are given. In this chapter, we studied a new kind of the divisor problem related to the nth co-efficient of the square of the derived zeta function. In a joint work with Makoto Minamide, we have derived the asymptotic formula for Riesz sum of order one for this new kind of the divisor function. As a result, we have deduced an asymptotic formula for the continuous mean value of error term. Also we have investigated the difference of continuous and discrete mean value of error term of order one and two respectively using Furuya's result. In the last chapter, the definition of square-free as well as k-free integers, their distribution, density and their application are introduced. Then a few results related to square free integers are described which is a joint work with Makoto Minamade. The last part of the chapter, deals with problems related to non k-free integers.

This thesis is about a study of some Lambert series. It is divided into three chapters.

In the zeroth chapter, we give some basic notations, definitions and few important results, which will be used throughout the thesis.

The first chapter is about a modular-type relation associated to Rankin-Selberg*L*-function. Zagier conjectured that the Lambert series

$$\sum_{n=1}^{\infty} \tau^2(n)e^{-nz}$$

should have an asymptotic expansion, when z $\to 0^+$, and it can be expressed in terms of the non-trivial zeros of the Riemann zeta function. Hafner and Stopple proved this conjecture. We have tried to generalise this result for any cusp form for the full modular group. We have mainly studied the Rankin-Selberg*L*-function and the symmetric square *L*-function associated to a cusp form and their corresponding functional equations, due to Rankin and Shimura. Using the relation between these two *L*-functions, we have derived an asymptotic expansion of the Lambert series

$$\sum_{n=1}^{\infty} c^2(n)e^{-nz}$$

in terms of the non-trivial zeros of the Riemann zeta function, when z $\to 0^+$, where c(n) is the n-th Fourier coefficient of a cusp form over the full modular group.

The last chapter is about the study of cotangent and secant zeta functions and their generalizations. Recently, Lalin, Rodrigue and Rogers have studied the secant zeta function and its convergence. They found many interesting values of the secant zeta function at some particular quadratic irrational numbers. They also gave modular transformation properties of the secant zeta function. We have generalised the secant zeta function as a Lambert series and proved a generalised result for Lambert series, from which the main result of Lalin et al. follows as a corollary. In this work we used the theory of generalised Dedekind eta-function, developed by Lewittes, Berndt and Arakawa.

The study of the local and global well-posedness of nonlinear evolution PDE in spaces of lowregularity represents one of the most active research fields, where the deepest machinery of modernharmonic analysis is applied. The principal aim of this PhD dissertation is to study nonlinearSchrödinger, wave and Klein-Gordon equations in the case of modulation $M^{p},{}^{q}(\mathbb{R}^{d})$ and Wieneramalgam $W^{p},{}^{q}(\mathbb{R}^{d})$ (time-frequency) spaces.

In the last decade, many mathematicians have used these spaces as a regularity class for the Cauchyproblem. In fact, fantastic progress have been done in the last decade from the PDE point of view inthese spaces. But some of the fundamental issues were left open by active researchers in this field.For instance: (1) Whether one can take power type nonlinearity $u|u|^{\alpha}$ (α $(0,\infty)\backslash 2\mathbb{N}$) in Schrödingerequation to obtain local well-posedness result? (2) The global well-posedness for the NLS withinitial data (large) in modulation spaces has not yet clear due to lack of any useful conservationlaws in these spaces by which one can guarantee global well-posedness.

We obtain some sufficient conditions for nonlinearity uF(u) and |u| to be in $M^{1},{}^{1}(\mathbb{R})$ whenever u $M^{1},{}^{1}(\mathbb{R})$ and F is a contraction on $\mathbb{C}$.

We study the Cauchy problem for Hartree type equations, that is, Schrödinger equations with cubicconvolution nonlinearity $F(u)=K \ast |u|^2$ under a specified condition on the potential K with Cauchydata on modulation spaces. We have established local and global well-posedness results for theHartree type equations.

In fact, these time-frequency spaces are present in various problems in the analysis, which alsoinvolves the study of twisted convolution. Finally, we take an excursion to the study of factorizationproblems with respect to twisted convolution in the realm of time-frequency and Lebesgue spaces.We have also illustrated its applications to functional analysis.

This thesis involves problems related to elliptic curves, Diophantine equations and number sequences. The first problem is about classifying a family of elliptic curves over rationals which have rank zero over number fields. In fact, we give the information about a necessary and sufficient condition for elliptic curves over rationals which are having rank zero over number fields.

The second result is about computing torsion subgroups over number fields for a family of elliptic curves over the rationals. In fact, we compute explicitly torsion subgroups over a class of number fields.

The third problem is about finding an upper bound for the maximal length of an arithmetic progression in coordinates of points on a family of elliptic curves. The construction of points on a family of elliptic curves over the rationals which are in arithmetic progression has been done.

The fourth problem is about finding out the perfect powers in a product of terms which are coming from certain number sequences like sequnce of balancing numbers and Lucas balancing numbers. We also give information about solving a recent conjecture on Diophantine equation using properties of Lucas balancing numbers.

The final result is about finding an upper bound for the length of an arithmetic progression which is represented by an integral binary quadratic form whose discriminant is not a perfect square. We also give information about the representation of three term arithmetic progression by an integral binary quadratic form.

The thesis consists of two themes, Euler's constant and Identities involving multiple zeta values. In the first part, we consider a generalisation of the classical Euler's constant. A special case of these constants was first introduced by Briggs and the notion was later discussed by Lehmer again after which they are known as the Briggs-Lehmer constants. We link these constants to generalised Briggs-Lehmer constants. We discuss the question of transcendence of these generalised numbers.

We have shown an identity involving generalised Euler-Briggs constants, Euler's constant and linear forms in logarithms. This generalises as well as gives an alternate proof of an identity of Lehmer.Further, this identity facilitates an investigation of the (conjectural) transcendental nature of generalised Euler-Briggs constants. Investigations of similar type were carried out in a joint work with Gun and Saha in 2014, which involved the interplay between additive and multiplicative characters. This in turn rendered inevitable a careful analysis of multiplicatively independent units in suitable cyclotomic fields. The generalised Lehmer's identity derived here avoids this leading to natural and transparent proofs of the earlier works. It also allows us to prove a stronger result.

The importance of these results is to get information about the nature of the Euler's constant that is if we have an element in the set which is algebraic other than the Euler constant then we can explicitly conclude that the Euler's constant is transcendental.

In the second part, we generalised identities involving Hurwitz zeta function, multiple zeta values proved by I. Mezo and show that these are transcendental numbers.

5.2 Institute of Mathematical Sciences (IMSc), Chennai

During the period, 11 students were awarded Ph.D. degree in Mathematics. Highlights from some the theses are presented as follows.

Let sl_2(t) denote the current algebra of the complex Lie algebra sl_2. Chari and Pressley have introduced bases for local Weyl modules of sl_2(t). Some results regarding the `stability' of these bases are first presented. Introducing the notion of a partition overlaid pattern (POP), a notionof area is introduced and some results are obtained on area maximizing Gelfand-Tsetlin patterns. Then a bijection is established between coloured partitions and POPs. A conjecture about the stability of Chari-Loktev bases is presented as arevarious results on the triangularity of Gelfand-Tsetlin and Chari-Loktev bases forrepresentations of sl_r.

Given a finite dimensional Hopf algebra H, a certain natural inclusion of infinite iterated crossed product algebras A ⊆B is associated to it and it is then shown that B is the crossed product (also known as the smash product in Hopf algebra literature) of A by D(H) where D(H) is the Drinfeld double of H. More significantly, it is shown that D(H) is the only finite-dimensional Hopf algebra with this property, thus producing a context in which the Drinfeld double arises very naturally.While proving this, an explicit embedding of D(H) into the triple iterated crossedproduct is established which might be regarded as a map from P_(2,+)(D(H))to P^(2)_(2,+)(H∗) . It is thus a natural question to ask whether this embeddingmay be extended to a planar algebra map from P(D(H)) to P^(2)(H∗). This is answered in the affirmative thus obtaining an injective planar algebra homomorphism from P(D(H)) to P^(2)(H∗) whose image is also characterised.

Let D(l,s) be the Demazure modules of the current algebra sl_2(t). A recursive formulae is established for the multiplicities of Demazure modules in the level m-Demazure flag of level-l Demazure modules for any m ≥ l ≥ 1. A generating series which encodes the multiplicities of level m Demazure modules inside a level l Demazure module for any m ≥ l ≥ 1 is defined. An explicit formula for this generating series is given when l=1 for arbitrary m and it is proved that they are actually rational functions involving Chebyshev Polynomials. Since level 1 Demazure modules are local Weyl modules, this result completely determines the numerical multiplicities of a level m-flag of a local Weyl module for any given m ≥ 1. Another main result concerns the q-multiplicities when l=1 and m=3. It is proved that when the generating functions of those q-multiplicities are specialized, they reduce to expressions involving the fifth order mock theta functions of Ramanujan.

This thesis considers fluctuations of error terms appearing in various asymptoticformulas. In this thesis, some classical methods that give magnitude of fluctuations of these error terms are revisited and modified to obtain the Lebesgue measure of the sets where these fluctuations occur. This generalises a theorem due to Kaczorowski and Szyldo, and a theorem due to Bhowmik, Ramare and Schlage-Puchta. A new application of this method to the error term in Prime Number Theorem is demonstrated and a result which is very close to the conjectural result is obtained. Some applications to error terms appearing in average order of a twisted divisor function, and the square-free divisors are also given. A study of the influence of measure of the sets where the error term is large to its fluctuations of comparable magnitude is also undertaken.This approach generalises a method due to Landau and is used to prove some conditional oscillation results to the error term appearing in the average order of non-isomorphic abelian groups, and average order of a twisted divisor function. Moreover, the very general set-up of this method allows several other applications.

After some preliminaries, this thesis introduces the Anderson model along with someimportant results related to the spectral structure of a certain class of random operators. The main result of thesis is proved in a series of steps. First it is shown that the set of certain w where the analysis fails is of measure 0. Then the absolutely continuous part of the measure is analysed by reducing it to a matrix problem.In case of the trace measure, this problem is handled by solving it for two perturbations. Finally, for the multiplicity results, equivalence of the trace measure is used and cyclic vectors for each of the Hilbert subspaces for the singular part of the measures are identified.

The thesis begins by discussing the possible transcendental nature of the generalised Euler-Briggs constants. This is followed by a study of the linear independence of these over the field of rational numbers as well as over other number fields and the field of algebraic numbers. A non-trivial lower bound on the dimension of certain vector spaces generated by these constants is derived. Some results are obtained on the algebraic independence of these generalised Euler-Briggs constants. These results are conditional, subject to the weak Schanuel conjecture. Finally, the connection between the generalised Euler-Briggs constants and certain infinite series is explored. Inspired by a result of Lehmer, a necessary and sufficient condition for the existence of periodic Dirichlet series at s = 1 twisted by a certain principal Dirichlet character is obtained. This sum is expressed as a linear combination of generalised Euler-Briggs constants. As a result about the special values of a shifted periodic Dirichlet series is also proved, which can be seen as a variant of the Hurwitz zeta function.

The thesis begins by deriving translation formulas and thereby the meromorphic continuation of certain families of Dirichlet series along the line of Ramanujan. Then, the analytic properties of the multiple zeta functions are discussed. Translation formulas for these functions are obtained and then written in terms of infinite matrices to obtain a matrix formulation. The meromorphic continuation of the multiple zeta functions is also deduced by means of such a translation formula and induction on the depth. The matrix formulation is used to write down an expression for residues along the possible polar hyper planes and study the non-vanishing of these residues. Next, multiple Hurwitz zeta functions are considered. and translation formulas for these are derived. The meromorphic continuation is deduced and a list of possible singularities is derived. Using a fundamental property of the zeros of the Bernoulli polynomials the exact set of singularities of the multiple Hurwitz zeta functions is then determined. Next, multiple Dirichlet series associated to additive characters are considered and their meromorphic continuations are derived as well as their exact list of polar singularities. It is shown that the multiple Dirichlet series associated to additive characters are related to the multiple Dirichlet L-functions. Using such relations, meromorphic continuations are derived and possible list of polar singularities for multiple Dirichlet L-functions. Finally, a weighted variant of the multiple zeta functions is dealt with. Study of this weighted variant is not esoteric. It is shown that this weighted variant has some rich arithmetic structures and their location of singularities have an uniform pattern.

This thesis studies compact quantum groups from various viewpoints, with one of the major tools being the study of their automorphisms. It begins with an exposition of some known results in the theory together with some new results on automorphisms of compact quantum groups and on approximation properties, in particular, weak amenability and Haagerup property, of quantum groups. Next, the notion of "inner automorphisms" of compact quantum groups is introduced and the topological properties of the group of inner automorphisms of a compact quantum group are studied. It is shown that any normal quantum subgroup of a compact quantum group is stable under the action of any given "inner automorphism". However, by means of explicit examples, it is shown that the converse is false in general. Then the center of a compact quantum group is defined and studied. It is shown that if two given compact quantum groups have isomorphic fusion rules, then their centers are also isomorphic. This result is then used to compute the center of several examples. Actions of discrete groups on compact quantum groups are then studied. Various spectral properties of these non-commutative dynamical systems (which are referred to as CQG dynamical system in the thesis), like ergodicity, weak mixing, mixing, compactness, etc are studied. Combinatorial characterizations of these spectral properties are obtained and then used to give explicit examples of CQG dynamical systems which possess these properties. Furthermore, a structure theorem of general CQG dynamical systems, under mild conditions, is established by means of showing the existence and uniqueness of the maximal ergodic normal subgroup of a given CQG dynamical system. Finally, a comprehensive study of the bicrossed product and the crossed product constructions of compact quantum groups is carried out. The representation theory of these quantum groups are determined and used to study various approximation properties for these quantum groups, like weak amenability, (relative) Haagerup Property, (relative) Property (T), rapid decay, etc. In particular, a countable family of mutually non-isomorphic quantum groups possessing Property (T) is constructed. These are the first examples of non-trivial quantum groups, possessing Property (T).

The thesis includes results on two different themes: Algebraic complexity theory, and Fourier-analysis of Boolean functions. In the first part, completeness and reductions in algebraic complexity are revisited. Several arithmetic classes are characterised using polynomials whose monomials enumerate homomorphisms between two graphs. This includes the first natural circuit-independent family complete for algebraic P. Polynomial families that are of intermediate complexity under reasonable assumptions are obtained. The expressivity of the permanent polynomial is explored; it is shown to be quite expressive even when restricted to symmetric matrices, but is also shown to be exponentially weak with respect to monotone projections. It is shown that exponential boolean sums add no power in multilinear settings. In the second part, the Fourier-Entropy Influence Conjecture isdiscussed, and possible approaches towards a solution of it are explored. Upper bounds on Fourier entropy are obtained in special cases, yielding new results as well as new independent proofs of known results.

This thesis explores some non-group-theoretic approaches to the graph isomorphism problem. The power and limitations of these approaches towards isomorphism testing are evaluated. Using techniques from geometry and lattices, faster algorithms for a geometric analogue of graph isomorphism - formally called geometric graph isomorphism - are obtained. Then the problem of computing canonical forms for geometric point-sets is considered. The one-dimensional version of the Weisfeiler-Leman algorithm is commonly known as Color-Refinement, or naive vertex-classification. Colour-Refinement is a classical procedure used to distinguish non-isomorphic graphs. This motivates the following natural question: what is the exact scope of applicability of color-refinement? We call a graph G amenable if colour-refinement successfully distinguishes G from any other non-isomorphic graph H. A polynomial time algorithm for testing whether a given graph is amenable is obtained. Continuing this theme, the power and limitations of convex optimization techniques for graph isomorphism are then examined. In this context, there exists a very natural class of graphs called compact graphs for which the isomorphism problem can be efficiently solved using linear programming methods. It is shown that the class of compact graphs contains the class of amenable graphs. Exploring this connection further a strict hierarchy of graph classes based on structural, group-theoretic and algorithmic properties of graphs with respect to isomorphism testing is studied.

Propositional proof complexity is an extensively studied area, with a number of lowerbound techniques for various propositional proof systems. This thesis assesses whether similar techniques are applicable for proof systems for quantified Boolean formulas (QBFs). The major contributions of this work are as follows: (1) It is shown that level-ordered Q-resolution and tree-like Q-resolution, two restrictions of Q-resolution systems, are incomparable. (2) The feasible interpolation technique is established for all CDCL-based QBF Resolution calculi. This provides the first general lower bound method for CDCL-based QBF calculi and also extends the scope of the feasible interpolation technique. (3) A cutting planes system CP+\forall~red for QBFs is introduced and the proof-theoretical strength of this new calculus is analysed. Strategy extraction technique and feasible interpolationtechnique for the new calculi are also established. (4) It is shown that both the size-width relation and the space-width relation for Resolution proof systems drastically fail in Q-resolution, even in its weaker tree-like version.

5.3 National Institute for Science Education and Research (NISER), Bhubaneswar

During the period, one student was awarded Ph.D. degree in Mathematics. Highlights of the thesis are presented as follows.

Modular forms and Dirichlet series are important objects in number theory and it has a wide range of applications in all other branches of Mathematics as well as in Physics. Kohnen [1991] constructed certain cusp forms whose Fourier coefficients involve special values of certain Dirichlet series of Rankin type by computing the adjoint map w.r.t. the Petersson scalar product of the product map by a fixed cusp form. Using differential operators one can define certain bilinear operators called the Rankin-Cohen brackets which is generalization of product. Recently the work of Kohnen has been generalized by Herrero [2015], where the author computed the adjoint of the map constructed using Rankin-Cohen brackets instead of product by a fixed cusp form. Fourier coefficints of the image of a cusp form under the adjoint map involves special values of certain Dirichlet series of Rankin-Selberg type similar to the one which appeared in the product case with certain twisting arising from binomial coefficients appearing in the Rankin-Cohen bracket. Rankin-Cohen brackets for Jacobi forms and Siegel modular forms of genus two were studied by Choie, Eholzer [1997, 1998] explicitly using certain differential operators. The main objective of this thesis is to extend the work of Herrero to the case of Jacobi forms, Siegel modular forms of genus two and modular forms of half integral weight.

Section-III

Synopses of completed Ph.D. theses during 2016-17

1. Name : **Soumen Ghosh**
Enrolment No. : PHYS06200904002
Date of Award of degree : 05.04.16
Constituent Institute : Institute For Plasma Research
Title : Study Of Localized Potential Structure And Heating In Expanding Helicon Plasma

Abstract

Spontaneous formation ofelectrostatic potential structure has important role in electric propulsion. Double layer like potential structures are very common in space plasma due to earth diverging magnetic field. These structures are also observedin laboratoryexperiments. Thesis highlights observationsof non-uniform potentialsin geometrically expanding helicon plasma inassociation with diverging magnetic fields. Observation of multiple ion beams indirectly indicatedthe formation of multiple double layer like structures in other experiments. However, there is no direct evidence for theformation of multiple double layerlike structures, in an expanding helicon plasma systems. Thiswork presents a direct evidence of multiple axial potential structures (MAPS) inexpanding helicon plasma system. It is concluded from this work that the magnetic field topology dictates the physics of downstream helicon plasma which is responsible for the formation of this potential structures. It is observed that the electrons are locally heated up axially away from the antenna center which is not due to near antenna fields. Further downstream from the location of the localized electron heating density rises.These localized electron heating and downstream density riseobservation is critically analyzed and find out as a cause for the formation of non-uniform potential structures. Inhomogeneous radial density distribution after the expansion may reduce the efficiency of plasma acceleration, which causes due to rotational kinetic energy conversion into axial kinetic energy in a diverging system. Independent role of magnetic and geometrical aperture on radial density inhomogeneity is studied. In this PhD thesis, experimental results with comprehensive analysis with physics based modellingare discussed to explain the localized potential structure, electron heating and downstream inhomogeneity observed in expanding *he*licon *ex*perimental (HeX) system.

Publications

Journal:

1. Localized electron heating and density peaking in downstream helicon plasmaSoumen Ghosh, K. K. Barada, P. K. Chattopadhyay, J. Ghosh, and D. Bora.Plasma Sources Sci. Technol. 24, 034011, (2015).
2. Resolving an anomaly in electron temperature measurement usingdouble and triple Langmuir probesSoumen Ghosh, K. K. Barada, P. K. Chattopadhyay, J. Ghosh, and D. Bora. Plasma Sources Sci. Technol. 24, 015017, (2015).
3. RF compensation of single Langmuir probe in low density heliconplasmaSoumen Ghosh, P. K. Chattopadhyay, J. Ghosh, and D. Bora.Under reviewfor publication in Fusion Engineering and Design.
4. Role of magnetic aperture in downstream annular plasma formationSoumen Ghosh, P. K. Chattopadhyay, J. Ghosh, and D. Bora.To be submitted for publication in refereed journal.
5. Formation of multiple axial potential structures (MAPS) in expanding helicon plasmasSoumen Ghosh, P. K. Chattopadhyay, J. Ghosh, and D. Bora.To be submitted for publication in refereed journal.

Conferences:

1. A novel gridded retarding field energy analyzer for IEDF measurementSoumen Ghosh, P. K. Chattopadhyay, J. Ghosh, and D. Bora.*42nd EPSConference on Plasma Physics, 22-26 June 2015, Lisbon, Portuga*

2. Name : **Apurba Kheto**
Enrolment No. : PHYS05201104002
Date of Award of degree : 05.04.16
Constituent Institute : Saha Institute of Nuclear Physics,
Title : Isospin Dependent Entrainment In Rotating Superfluid Neutron Stars.

Abstract

The main theme of the thesis entitled "Isospin Dependent Entrainment in Rotating Super-fluid Neutron Stars" is to describe the effects of isospin on the entrainment and equilibrium structure in superfluid neutron stars using realistic equations of state in the Walecka model including rho mesons and scalar self-interaction. In the first part of the thesis we have focused on the entrainment effect between superfluid neutrons and charge neutral fluid (called the proton fluid) which is made of protons and electrons in neutron star interior within the two-fluid formalism and using a relativistic model where baryon-baryon interaction is mediated by the exchange of sigma, omega and rho mesons. This model of strong interaction also includes scalar self interactions. Neutron star matter is highly asymmetric in neutron and proton number densities. The inclusion of rho-meson takes care of the isospin effect in neutron star matter. For the calculation of the entrainment we have chosen neutron star configurations which are just below maximum masses . We estimated dynamical neutron and proton effective masses for these two parameter sets of Glendenning (GL) and another non-linear (NL3) interaction and found that the neutron effective mass increases with density and becomes greater than the free neutron mass in both cases and proton effective mass decreases with density initially and rises with density later. We have calculated the Landau effective mass for nucleons and found that neutron and proton effective masses decrease as baryon density increases for both parameter sets, and they are below their bare masses. The entrainment parameter calculated using two parameter sets remains constant in the core and drops rapidly at the surface. We have found an appreciable difference between two results towards the centre. We have compared this result with that of the situation excluding rho mesons and it is clear that the inclusion of rho mesons strongly enhances the entrainment parameter. We have also compared our results with those of the relativistic Landau Fermi liquid theory and found appreciable differences.In the later part of the thesis we have explored for the first time the effects of the isospin dependent entrainment and the relative rotation between two fluids on the global properties of slowly rotating superfluid neutron stars, such as the structures and Kepler limit in the two-fluid formalism. In this calculation we have used the Hartle's slow rotation approximation to Einstein's field equation so that the equations governing rotating neutron stars in the slow rotation approximation are second order in rotational velocities of neutron and proton fluids. It is noted that the corrections to the proton number density are significantly modified in the presence of rho mesons. We have also calculated the rotationally induced deformation of the star in terms of the ratio of the polar and equatorial radii by considering the proton rotation rate to be equal to that of the fastest rotating pulsar having spin frequency 716 Hz. The non-rotating situation is achieved when the relative rotation rate approaches zero. When ratio of relative rotation rate is less than unity , the Kepler frequency monotonically increases with decreasing relative rotation rate whereas the opposite scenario was found in the work of Comer. It is noted that the Kepler limit obtained with the isospin dependent entrainment effect is lower than that of the case when the isospin term is neglected in the entrainment effect.

Publications

Journal

1. Slowly rotating superfluid neutron stars with isospin dependent entrainment in a two-fluid model. Apurba Kheto and Debades Bandyopadhyay;Physical Review D 91, 043006 (2015).
2. Isospin dependence of entrainment in superfluid neutron stars in a relativistic model.Apurba Kheto and Debades Bandyopadhyay;Physical Review D 89, 023007 (2014)

3. Name : **Lumbini Ramraj Yadav**
Enrolment No. : LIFE09200804002
Date of Award of degree : 05.04.16
Constituent Institute : Tata Memorial Centre
Title : Structural And Functional Approaches To Evaluate Novel Missense Germline Mutations In Brca1.

Abstract

BRCA1 is a pleiotropic tumour suppressor gene with autosomal dominant inheritance. BRCA1 performs the function of DNA repair, transcription activation and repression. Deleterious germline missense variants in BRCA1 are responsible for increased risk of hereditary breast and ovarian cancer. While frameshift and truncating mutations are pathogenic, it is not possible to predict the clinical significance of the missense VUS (variant of uncertain significance) without comprehensive analysis. The aim is to characterize the missense VUS reported in TMC cohort using clinicopathological, *in silico*, biophysical and structural approaches. 19 missense variants of BRCA1 identified from 48 Indian families were classified into different IARC class based on their posterior probability values. Three novel variants belonging to pathogenic class were further comprehensively characterized based on functional, biophysical and structural methods. Studies on BRCA1 central fragments revealed that these regions are intrinsically disordered. To study ligand induced folding of central fragment of BRCA1 (502-802) with DNA suggested a change in the hydrodynamic radius, folding pattern. Our study on ZBRK1 (206-424) amino acids suggests that it forms a homotetramer and binds ds DNA with a stoichiometry of 1:2, in absence of zinc. The study on different fragments in C-terminal of BRCA1 indicates that BRCA1 BRCT is stable domain. BRCA1 (1560-1859) was crystallized and its structure was refined up to 4.0 Å resolution but no electron density was visible for residues upstream of (1646-1859) amino acids. Purification and structure solution data indicate the interesting possibility that BRCA1 (1560-1859) is autolytic but it needs further confirmation.

Publications

Journal

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2. "Functional assessment of intrinsic disorder central domains of BRCA1." LumbiniR.Yadav, SharadRai, M.V.Hosur, & Ashok K. Varma. Journal of Biomolecular Structure and Dynamics, 2015, DOI:10.1080/07391102.2014.1000973.
3. "Structural basis to characterise transactivation domain of BRCA1." Lumbini R. Yadav, Mahamaya N. Biswal, M.V. Hosur , NachimuthuSenthil Kumar and Ashok K. Varma. Journal of Biomolecular Structure and Dynamics, 2016.
4. "Structural and functional characterization of transactivation Domain of BRCA1." Lumbini R. Yadav, Ashok K. Varma. ActaCrystallographica Section A, 2011, A67, C221-C222.

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2. Preliminary crystallographic studies of BRCA1 BRCT-ABRAXAS complex. Badgujar DC, Sawant U; Vikrant, Yadav L, Hosur MV, Varma AK. ActaCrystallographica. Section F, Structural Biology Communications, 2013, F69, 1401–1404.
3. Structural and functional implication of RAP80 ΔGlu81 mutation Vikrant, Kumar R, Yadav LR, Nakhwa P, Waghmare SK, Goyal P,Varma AK. PLOS One. 2013.

4. Name : **Ashutosh Mishra**
Enrolment No. : ENGG02201104012
Date of Award of degree : 05.04.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Thermal Ratcheting Of Thin Shells: Significance Of Thermomechanical Interactions.

Abstract

The phenomenon of progressive deformation with increase in plastic strains cycle by cycle, such that collapse or failure of the structure occurs after gross plastic deformation, is termed as *Ratcheting*. Moreover, ratcheting in a cylindrical shell subjected to cyclic axial thermal gradients due to moving temperature front, with and without mechanical load, is a special category, termed as *Thermal ratcheting*. Thermal ratcheting in the main vessel of Sodium cooled Fast Reactors (SFR) occur due to sodium free level variations. Thermal ratcheting can cause dimensional instability due to excessive deformation beyond allowable limits prescribed by the design codes. Additionally, the accumulated inelastic strain in radial direction may affect the movement of in-service inspection (ISI) system between the gap of the main vessel and the safety vessel that assess the extent of damage if any to keep it under control. Out of various constitutive models reported in literatures, no single model is robust enough to cover the various aspects of mechanics and metallurgy to accurately predict the realistic ratcheting behavior. Further, it is quite challenging to perform numerical analysis by implementing different user defined constitutive models. The present work addressed the thermal ratcheting behavior of smooth cylindrical shell using different constitutive models highlighting the significance of different loading methods. Simplified expressions for plasticity integration for time independent and dependent constitutive models have been proposed. This work also presents the experimental and numerical simulation of thermal ratcheting and significance of thermomechanical interaction is demonstrated for two-bar system and cylindrical shell. The present work includes a critical design aspect of main vessel of SFR for its safe and reliable operation.

Publications

Journal

1. A. Mishra, P. Chellapandi, R. Suresh Kumar and G. Sasikala. Effect of frequency of free level fluctuations and hold time on the thermal ratcheting behavior. *International Journal of Pressure Vessels and Piping.* 2015; 129–130: 1–11.
2. A. Mishra, P. Chellapandi, R. Suresh Kumar and G. Sasikala. Effect of Temperature Rate Term while Predicting Thermal Ratcheting of a Thin Cylinder due to Cyclic Temperature Variation. *Transactions of the Indian Institute of Metals.* 2015; 68: 161-169.
3. A. Mishra, P. Chellapandi, R. Suresh Kumar and G. Sasikala. Comparative study of cyclic hardening behavior of SS 316L using time independent and dependent constitutive modeling: A simplified semi-implicit integration approach*. Transactions of the Indian Institute of Metals.* 2015; 68; 623-631.
4. A. Mishra, R. Suresh Kumar, and P. Chellapandi. Progressive deformation behaviour of thin cylindrical shell under cyclic temperature variation using Combined Hardening Chaboche Model*. Latin American Journal of Solids and Structure.* 2014; 11:980-992.
5. A. Mishra, R. Suresh Kumar, G. Sasikala and P. Chellapandi. Influence of the frequency of level fluctuations with reference to progressive deformation of thin cylindrical shell. *Procedia Engineering* 2014; 86:95 –102.
6. A. Mishra, R. Suresh Kumar, and P. Chellapandi. Time dependent ratcheting of thin cylindrical shell due to axial temperature variation using visco-plastic model. *International Journal of Engineering and Technology.* 2014; 6: 234-237.

7. A. Mishra, Kulbir Singh, R. Suresh Kumar and P. Chellapandi. Experimental and numerical simulation of thermal ratcheting behavior with thermomechanical interactions. *International journal of Pressure vessels and Piping* (Under review).

Conference Presentations

1. A. Mishra, R. Suresh Kumar, G. Sasikala and P. Chellapandi. Significance of thermo-mechanical interaction in thermal ratcheting behavior. 7th International Conference on Creep, Fatigue and Creep-fatigue Interaction (CF-7), January 19-22, 2016, Indira Gandhi Centre for Atomic Research, Kalpakkam, India.
2. A. Mishra, P. Chellapandi, R. Suresh Kumar and G. Sasikala. Effect of Temperature Rate Term while Predicting Thermal Ratcheting of a Thin Cylinder due to Cyclic Temperature Variation. International Symposium for Research Scholars on Metallurgy, Materials Science and Engineering (ISRS-2014), Dec-11-12, 2014, IITM, India.
3. A. Mishra, R. Suresh Kumar, G. Sasikala and P. Chellapandi. Influence of the frequency of level fluctuations with reference to progressive deformation of thin cylindrical shell. First International conference on Structural Integrity (ICONS-2014), Feb-4-7, 2014, Kalpakkam.
4. A. Mishra, R. Suresh Kumar and P. Chellapandi. Shakedown study of thin cylindrical shell due to moving temperature distribution using Combined Hardening Chaboche Model. Indian Conference on Applied Mathematics (INCAM 2013), 4th-6th July 2013, IIT Madras, India.
5. A. Mishra, R. Suresh Kumar and P. Chellapandi. Simulation of Thermal Ratcheting of thin cylindrical shell due to moving temperature distribution using Combined Hardening Chaboche Model. International Conference on Pressure Vessel and Piping (OPE 2013), 13th-16th February, 2013, Mamallapuram, Chennai, India.

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5. Name : **Shikha Sharma**
Enrolment No. : CHEM01200904012
Date of Award of degree : 05.04.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Synthesis Of Novel Extractants For Back-End Fuel Technology

Abstract

This thesis describes design, synthesis and extraction evaluation of new organic molecules called extractants for separation of metal ions contained in nuclear waste solutions. The content of the thesis have been divided into five chapters.An introduction of back end of nuclear fuel cycle along with a comprehensive literature survey on extractant used for separation of metal ions contained in nuclear waste have been presented in Chapter 1. Chapter 2 encloses the design, synthesis and extraction properties of a new class of ammonium based anion exchangers embedded with a terminal α-dialkylamino *N*,*N*-diisobutylacetamide group for separation of oxometalates. The role of amide group in extraction from relatively higher concentration of nitric acid medium has been evaluated. Two different inorganic-organic hybrid polyoxomolybdate complexes have been synthesized and their X-Ray crystallographic characterization has been studied in detail. Comparative study of hydrolytic and radiolytic degradation behavior of deuterated TBPs (d_n-TBPs) and undeuterated TBP has been discussed in chapter 3. Synthesis of *d*-labelled TBPs, deuterated at four different positions has been achieved with good isotopic purity and yields. The isotope effect was found to be minimal in this γ radiolytic degradation study. Chapter 4 contains design and synthesis of three conformationally constrained bridged oxa-diamide ligands and evaluation of their extraction behaviour for Am(III), Eu(III), Pu(IV), U(VI) from the nitric acid medium using solvent extraction and membrane separation techniques. This chapter also includes design, synthesis and solvent extraction studies of a Pu selective rigidified oxa-diamide. Chapter 5 comprised of design and synthesis of a new class of quaternary ammonium iodide based ligands with 2-(*N,N*-diisobutyl)acetamide as an alkyl appendage for separation of Ru from nitric acid medium. Extraction behaviour of these extractants for ruthenium has been studied in detail by solvent extraction as well as solid phase extraction technique. The extractant showed selective extraction of ruthenium from HNO_3 medium. The role of iodide ion was found to be interesting in extraction process.

Publications

Journal

1. "Comparative studies on radiolytic degradation of deuterium labeled and unlabeled tributyl phosphates", Shikha Sharma, Sunil K. Ghosh, Devidas B. Naik, Prem S. Dhami, Joti N. Sharma, J. Radioanal. Nucl. Chem., 2014, 302, 583-591.
2. "α-Dialkylamino N,N-diisobutylacetamides: a new class of anion exchanger with intramolecular buffering properties", Shikha Sharma, Sunil K. Ghosh, Anitha M, Joti N. Sharma, RSC Adv., 2014, 4, 27837-42.
3. "Dialkylmethyl-2-(N,N-diisobutyl)acetamidoammonium iodide as a ruthenium selective ligand from nitric acid medium", Shikha Sharma, Sunil K. Ghosh, Joti N. Sharma, J Hazard. Mater., 2015, 295, 17-21.
4. "Design, synthesis and extraction studies of a new class of conformationally constrained (N,N,N',N'-tetraalkyl) 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxamides", Shikha Sharma, Surajit Panja, A. Bhattachariya, Prem S. Dhami, Preetam M. Gandhi, Sunil K. Ghosh, Dalton Trans., 2015, 44, 12771-12779.
5. "Synthesis and characterization of two different inorganic-organic hybrid isopolyoxomolybdates with α-dipropylammonium N,N-diisobutylacetamide by varying reaction conditions", Shikha Sharma, Sunil K. Ghosh, Mukesh kumar, Joti N. Sharma, Polyhedron, 2015, 100, 290-295.
6. "Efficient transport of Am(III) from nitric acid medium using a new conformationally constrained (N,N,N',N'-tetr-2-ethylhexyl) 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxamide across a Supported Liquid Membrane", Shikha Sharma, Surajit Panja, Prem S. Dhami, Preetam M. Gandhi, Sunil K. Ghosh, J. Hazard. Mater., 2016, 305, 171-177.
7. "Synthesis and Extraction Studies with a Rationally Designed Diamide Ligand Selective to Actinide(IV) pertinent to Plutonium Uranium Redox Extraction Process, Shikha Sharma, Surajit Panja, A. Bhattachariya, Prem S. Dhami, Preetam M. Gandhi, Sunil K. Ghosh, Dalton Trans., 2016, 45, 0000-0000 (DOI: 10.1039/C6DT00748A).
8. "Sorption of ruthenium by dipropylmethyl-2-(N,N-diisobutyl)acetamide ammonium iodide impregnated Amberlite XAD-4 resin from nitric acid medium", Shikha Sharma, Sunil K. Ghosh, Joti N. Sharma, Sep. Sci. Technol., 2016, 0000-0000 (DOI:10.1080/01496395.2016.1142563)

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1. Synthesis of deuterium labeled tributyl phosphates as radiation stable nuclear extractants. Shikha Sharma, Sunil K. Ghosh, in the Proceedings of conference *ISMC-2013* held in BARC, Mumbai during Dec 9-13, 2012.
2. Radiolytic degradation studies on deuterium labeled and unlabeled tributyl phosphates. Shikha Sharma, S. K. Ghosh, D. B. Naik, P. S. Dhami, J. N. Sharma, in the Proceedings of conference *TSRP-2014* held in BARC, Mumbai during, Jan 6-9, 2014.
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4. Synthesis of stable and selective nuclear extractants for back end fuel technology, Shikha Sharma, S. K Ghosh, in the Proceedings of conference *RSM-2014* held in CKT College, Mumbai during, Feb 21-22, 2014.

5. Solvent extraction evaluation of novel bi-functional extractants α-dialkylamino *N,N'*-diisobutylacetamides: An anion exchanger with intramolecular buffering properties, Shikha Sharma, S. K. Ghosh, Anitha M, J. N. Sharma, in the Proceedings of conference *SESTEC-2014* held in BARC, Mumbai during, Feb 25-28, 2014
6. α-Dialkylamino *N*,*N*-Diisobutylacetamides as a New Class of Anion Exchanger with Intramolecular Buffering Properties, , Shikha Sharma, S. K. Ghosh, Anitha M, J. N. Sharma, in the Proceedings of conference *ISMC-2014* held in BARC, Mumbai during, Dec 9-13, 2014.
7. Selective sorption of ruthenium from acidic medium by Amberlite xad-4 resin impregnated with iodide salt of *N*,*N* '-diisobutyl(α-trialkylammonium)-acetamide, Shikha Sharma, S. K. Ghosh, J. N. Sharma, in the Proceedings of conference *NUCAR-2014* held in BARC, Mumbai during, Feb 9-13, 2015.

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6. Name : **Dibyakrupa Sahoo**
Enrolment No. : PHYS10200904007
Date of Award of degree : 05.04.16
Constituent Institute : Institute of Mathematical Sciences,
Title : Investigating Violations Of Some Fundamental Symmetries Of Nature Via Dalitz Plots And Dalitz Prisms.

Abstract

The immensely familiar but subtle concept of symmetry pervades our deepest understanding of Nature and is central to contemporary mathematics and physics. This thesis looks at some of the fundamental symmetries of Nature which are revealed in the realm of elementary particles and investigates how violations of these symmetries can be observed in some specific elementary particle processes. The symmetries that are analysed in this thesis are CP, CPT, Bose symmetry and SU(3) flavor symmetry, out of which CPT and Bose symmetry are known to be exact symmetries of Nature, and both CP and SU(3) flavor symmetry are known to be violated in Nature. In this thesis Idiscuss how violations of CP, CPT, Bose and SU(3) flavor symmetries in some three-body meson decays lead to an observable asymmetry in their Dalitz plots. I have listed the specific kind of threebody decay modes which can be used to probe CP, CPT, Bose symmetry and SU(3) flavor symmetry violations. The choice of the decays modes plays a crucial role in these investigations and they are chosen keeping an eye on the effects of the underlying symmety. It is observed that in some cases, the parent particle has no role to play in the signature of symmetry violation underconsideration. In such cases the method is extended to include multi-body decays as well as continuum production processes. This leads to the concept of 'Dalitz prism' which is indeed a generalization of the Dalitz plot. The said symmetry violations lead to an observable asymmetry in the Dalitz prism. The Dalitz prism is helpful even when initial state radiation and final state radiation are present. Since, the Dalitz prism is a storehouse of data, it would help in precise measurements of violations of CP, CPT and Bose symmetries. The method of employing bothDalitz plots and the new concept of Dalitz prism to study the said symmetry violations is a new,powerful and unique methodology for such studies.

Publications

Journal

1. Dibyakrupa Sahoo, Rahul Sinha, and N. G. Deshpande, "Model independent method for aquantitative estimation of SU(3) flavor symmetry breaking using Dalitz plot distributions",Physical Review D 91, 076013 (2015), arXiv:1502.07089 [hep-ph].

2. Dibyakrupa Sahoo, Rahul Sinha, and N. G. Deshpande, “Testing violations of Bose and CPTsymmetries via Dalitz plots and their prismatic generalizations”, Physical Review D 91,051901(R) (2015), arXiv:1409.5251 [hep-ph].
3. Dibyakrupa Sahoo, Rahul Sinha, N. G. Deshpande, and S. Pakvasa, “Technique to observedirect CP violation in D mesons using Bose symmetry and the Dalitz plot”, Physical Review D 89, 071903(R) (2014), arXiv:1310.7724 [hep-ph].
4. Arjun Menon, Tanmoy Modak, Dibyakrupa Sahoo, Rahul Sinha and Hai-Yang Cheng,“Inferring the nature of the boson at 125–126 GeV”, Physical Review D 89, 095021 (2014), arXiv:1301.5404[hep-ph].
5. Tanmoy Modak, Dibyakrupa Sahoo, Rahul Sinha, Hai-Yang Cheng and T.C. Yuan,“Disentangling the Spin-Parity of a Resonance via the Gold-Plated Decay Mode”,arXiv:1408.5665[hep-ph]. Accepted for publication in Chinese PhysicsC.

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7. Name : **Shubhashis Rana**
Enrolment No. : PHYS07200904002
Date of Award of degree : 05.04.16
Constituent Institute : Institute of Physics,
Title : Effect of Thermal Fluctuations on Classical and Quantum Systems at Small Scales.

Abstract

For meso-scopic regime internal energy of the system becomes equivalent to the surrounding thermal fluctuations. In this regime the thermodynamic quantities like work, heat etc. become stochastic quantity and their value depend on the particular phase space evolution of the system. However these thermodynamic quantities obey some universal rules, collectively known as fluctuation theorems (Fts), which is valid even beyond linear response regime. We have mainly focused on the extensions of FTs to different scenarios. We have obtained a new fluctuation relations for heat engines (FRHE) in time periodic steady state (TPSS). Carnot’s inequality for classical thermodynamics follows as a direct consequence of this fluctuation theorem even in TPSS. For the special case of the absence of hot bath we obtain the integral FT for total entropy and for no extraction of work we get the generalized exchange FT. Using framework of finite time stochastic thermodynamics, we have carried out an extensive analysis of single particle heat engines by manipulating a Brownian particle in a time dependent harmonic potential with time-dependent coupling to two heat baths. Thermodynamic quantities such as work, heat and stochastic efficiency exhibit strong fluctuations in TPSS. The fluctuations of stochastic efficiency dominates over the mean value even in the quasi-static regime. The phase diagrams for system operations are qualitatively different for inertial and over-damped regimes. In TPSS, there are several realizations where the system does not work as a heat engine. Such transient Second law violating realizations decrease as we increase cycle time. Hence for larger cycle times our system work more reliably as an engine. Some of our results differ qualitatively from earlier claims in the literature. We have also verified FRHE in TPSS. Based on trajectory dependent path probability formalism in state space, we have derived generalized entropy production FTs and JE for a quantum system in the presence of multiple measurement and feedback. This is in contrast to the formal approach based on projection operator and density matrices. We have obtained these results for both isolated system as well as the system being weakly coupled to a heat bath. The obtained entropy production FTs retain the same form as in the classical case. The inequality of second law of thermodynamics gets modified in the presence of information. These FTs are robust against intermediate measurements of any observable performed with respect to Von Neumann projective measurements as well as weak measurements. After that, we have analysed the fluctuation relations for work and entropy in underdamped and overdamped systems, when the friction coefficient of the medium is space-dependent. We find that these relations remain unaffected in both cases. For the overdamped system, the analysis is more involved, and a blind application of normal

rules of calculus would lead to inconsistent results. Finally we have observed bistability is a necessary but not a sufficient condition for observing stochastic resonance. It is observed in superharmonic (hard) potentials, but is not observed in subharmonic (soft) potentials, even through potential is bistable. However, in both soft and hard potentials, we have observed resonance phenomenon as a function of driving frequency.

Publications

Journal

1. The role of soft versus hard bistable systems on stochastic resonance using average cycle energy as a quantifier. S. Rana, S. Lahiri and AM Jayannavar. The European Physical Journal B 84, 323 (2011).
2. Fluctuation theorems in presence of information gain and feedback. S. Lahiri, S. Rana and A. M. Jayannavar. J. Phys. A: Math. Theor. 45, 065002 (2012) .
3. *Quantum Jarzynski equality with multiple measurement and feedback for isolated system. S. Rana, S. Lahiri and A. M. Jayannavar. Pramana 79, 233 (2012).
4. *Fluctuation relations for heat engines in time-periodic steady states. S. Lahiri, S. Rana and A. M. Jayannavar. J. of Phys. A: Math. and Theor. 45, 465001 (2012).
5. *Generalized entropy production fluctuation theorems for quantum systems. S. Rana, S Lahiri and A. M. Jayannavar. Pramana 80, 207 (2013).
6. *Fluctuation theorems in inhomogenious media under coarse graining. S. Lahiri, S. Rana and A. M. Jayannavar. Physics Letters A 378, 979 (2014).
7. Extracting work from a single heat bath - A case study on Brownian particle under external magnetic field in presence of information . P. S. Pal, S. Rana, A. Saha and A. M. Jayannavar. Phys. Rev. E 90, 022143 (2014).
8. *Single Particle Stochastic Heat Engine. S. Rana, P. S. Pal, A. Saha and A. M. Jayannavar. Phys. Rev. E 90, 042146 (2014).
9. Anomalous Brownian Refrigerator . S. Rana, P. S. Pal, A. Saha and A. M. Jayannavar. Physica A 444, 783 (2016).

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8. Name : **S. Vanna Perumal**
Enrolment No. : ENGG02201104005
Date of Award of degree : 05.04.16
Constituent Institute : Indira Gandhi Centre for Atomic Research
Title : Experimental Studies On Reductve Extraction Of Actinides From Molten Salt Under Highly Stratifying Conditions.

Abstract

In pyrochemical reprocessing, LiCl-KCl eutectic salt with wide electrochemical window is employed as the electrolyte for selective separation of the actinides. The separation of the actinides here is based on the difference in thermodynamic stability (reduction potential) of their chlorides. In the electrorefiner, very stable fission products are dissolved and accumulated in the molten salt whereas the actinide elements having intermediate stability are selectively electro transported and deposited on the cathode. The accumulation of fission products in the electrolyte salt enforces periodic cleaning in order to maintain the decontamination factor of the actinide which is accomplished by treating with an ion exchange resin (zeolite). Prior to the reconditioning of the electrolyte, the actinides present in the electrolyte are removed by Actinide drawdown process (ADDP). The objective this thesis work is to investigate actinide draw down process using natural U as the represenive. The proposed work involves designing an experimental facility to operate at high temperature ensuring the mixing of molten salt and Li-Cd alloy phase. The experiment needs to be carried out in an inert gas glove box because of the hygroscopic nature of the molten salt and the high reactivity of Li-Cd alloy towards oxygen. It is a continuous reductive liquid- liquid extraction operation wherein the molten salt is contacted with Li-Cd alloy phase containing lithium as the reducing agent. As the melting temperatures of the salt and alloy phases are high, the setup is designed to operate at 773K. The molten salt eutectic containing 0.5 wt % U is contacted with molten Li- Cd alloy phase (Li~ 300 ppm) at 723 K. The extraction was carried out by maintaining the flow rates of salt and cadmium phases at 25 ml/min each and the mixing was performed by a specially designed continuous contactor provided with 3- impellers. Extraction efficiency of up to 99 percent is obtained for uranium in typical runs.In addition to these complexities, the effect of large difference in density between the cadmium phase (8000 kg/m^3) and salt phase (1600 kg/m^3) that can lead to stratification of the phases is also investigated to understand the dispersion of the phases. Considering the difficulties in observing the dispersion at high temperature operation with molten materials, it is proposed to carry out the fluid dynamic studies under cold flow condition. The two phase solid -liquid system with relative difference in density varying from 0.13 to 0.63 is considered as the representative for the liquid-liquid dispersion. The minimum impeller speed required for solid-liquid dispersion is experimentally determined and a correlation is proposed to predict the impeller speed. The findings of this work are discussed here.

Publications

Journal

1. "Actinides drawdown process for pyrochemical reprocessing of spent metal fuel", S. Vannia Perumal, B. Prabhakara Reddy, G. Ravisankar, K. Nagarajan, *Radiochemica Acta*, 2015, *103(4)*, 287-292.
2. "Effect of impeller type and density difference on draw down of low density microsphere", S. Vannia Perumal, S. Jayanti, K. Nagarajan, *Chem. Eng. Res. Design,* Dec'2015,104 , 571-578.

Conferences

1. "Actinides drawdown process for pyrochemical reprocessing of spent metal fuel", S. Vannia Perumal, B. Prabhakara Reddy, G. Ravisankar, K. Nagarajan, SESTEC-2014, BARC, Mumbai, February 25-28, 2014

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9. Name : **Kamali K.**
Enrolment No. : CHEM02201004007
Date of Award of degree : 12.04.16
Constituent Institute : Indira Gandhi Centre for Atomic Research
Title : High pressure Raman spectroscopic studies on anomalous thermal expansion materials.

Abstract

Thermal expansion is an important property of solids for many industrial and practical applications. Most materials expand on heating, but some materials exhibit opposite behaviour, i.e., they contract upon heating, which is termed as negative thermal expansion (NTE). Thermal expansion (or contraction) can be isotropic or anisotropic. The anomalous thermal expansion properties of various materials falling under the category of low, zero and colossal thermal expansion are analyzed using high pressure Raman spectroscopy based on the values of Gruneisen parameters. First-principles calculations on some materials provide information of the nature and contribution of various phonon modes over the entire Brillouin zone and correlation with their corresponding thermal expansion coefficient. Phase stability of some compounds with pressure is confirmed using high pressure synchrotron X-Ray Diffraction. In low thermal expansion materials of sodium zirconium phosphate (NZP) family, anisotropic negative thermal expansion along the *a*-axis is found to be due to two low energy soft Raman modes corresponding to a combination of PO_4 tetrahedral librations and Zr translations and coupled rotation of ZrO_6 and PO_4 tetrahedra. Two high pressure transitions at 5 and 5.8 GPa observed in Raman spectroscopy were confirmed by high pressure XRD analysis indicating rhombohedral R3 structure at 5 GPa and orthorhombic Pbcn structure at 6.7 GPa. The above soft NTE modes are responsible for the first phase transition through a polyhedral tilt mechanism. Further, anharmonicity of various Raman modes of $AZr_2(PO_4)_3$,A=Na, K, Rb, Cs are compared to correlate with tunable thermal expansion coefficient. Prototypic NZP is found to be stable up to 32 GPa but compounds with larger cations amorphize at lower pressures. In zero thermal expansion material TaO_2F a reversible cubic to rhombohedral phase transformation onsets around 0.8 GPa and gets completed at 4.4 GPa with all four predicted normal modes corresponding to R-3c phase and retaining the structure up to 19 GPa. Temperature dependent Raman measurements showed that the intensities of Raman bands remain almost unchanged with rise in temperature indicating static disorder in TaO_2F. On the other hand, all four modes of disorder-free rhombohedral high pressure phase showed the usual hardening behavior with increase in pressure contributing to positive thermal expansion. Colossal thermal expansion material $KMn[Ag(CN)_2]_3$ exhibits negative pressure derivative of the shear elastic constant C_{44}, indicating anisotropic linear compressibilities and thermal expansion. This in turn implies that high pressure phase transformation arises due to shear instability. Coupled atomic displacement of two low energy optical modes with negative Gruneisen parameters exhibit dominant displacement of Ag atoms in $KMn[Ag(CN)_2]_3$, and are found to be responsible for the pressure induced phase transformation at 2.8 GPa. Pressure variation of mean partial phonon frequencies has suggested that large amplitude displacements of Ag atoms could occur with minimum enthalpy cost. The anisotropic linear compressibility and thermal expansion are facilitated by anharmonic lattice vibrations of Ag atoms. Comparison of phonon spectra of $KMn[Ag(CN)_2]_3$ and $Ag_3[Co(CN)_6]$ showed lattice stiffening of the former which renders the structure resistant to pressure induced phase transformation up to 2.2GPa.

Publications

Journal

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2. Linear compressibility and thermal expansion of $KMn[Ag(CN)_2]_3$ studied by Raman spectroscopy and first-principles calculations K. Kamali, T. R. Ravindran, C. Ravi, R. M. Sarguna, T. N. Sairam and G. Kaur, J. Phys. Chem. C, 117 (2013) 25704.
3. High pressure Raman spectroscopic study of TaO_2FK. Kamali, T. R. Ravindran and T. N. Sairam Vibrational Spectroscopy, 71 (2014) 12.
4. Pressure induced transformation in $NaZr_2(PO_4)_3$ studied by Raman spectroscopy and X-Ray diffraction K. Kamali, T. R. Ravindran, N. V. Chandra Shekar, K. K. Pandey, S. M. Sharma and J. Solid State Chem. 221 (2015) 285.
5. Comparative Raman spectroscopic study of phase stability and anharmonic effects in $AZr_2(PO_4)_3$ (A= K, Rb and Cs) K. Kamali, T. R. Ravindran and C. Ravi Spectrochim. Acta, Part A 155, (2016) 38.

10. Name : **Sushmita Chatterjee**
Enrolment No. : LIFE09200904014
Date of Award of degree : 12.04.16
Constituent Institute : Tata Memorial Centre
Title : Evaluation of sodium iodide symporter (hNIS) mediated targeted radioiodine therapy in breast cancer by non invasive imaging.

Abstract

NIS is a membrane glycoprotein that mediates active transport of Na^+ and I^- in the thyroid follicular cells for synthesis of thyroid hormones, and is a major target for radioiodine therapy in thyroid cancer patients. In the present Ph.D. research work, we evaluated NIS expression in a large number of breast cancer primary (181) and metastatic tumour tissue samples (45) by immunohistochemistry (IHC) and real time PCR. We observed upregulated NIS expression in primary as well as metastatic breast tumour tissues as compared to adjacent breast normal tissue used as control. A significant positive correlation of NIS with ER is observed, although association with other factors was not evident. Additionally we analyzed NIS expression in 59 primary breast tumour tissues by quantitative real time PCR using TaqMan assays. Our results suggest upregulated NIS expression and positive correlation between NIS and ER at the transcript level.Taking the study forward we developed a mammalian expressing plasmid vector for correlated expression of NIS and a reporter gene Turbofp. Fluc2. We have established unique cellular models based on few breast adenocarcinoma cell lines. Thorough analysis of the established cells showed consistent and correlated expression of the therapeutic and reporter gene over multiple passages. Extensive in detailed analysis of NIS expression in various clones showed 2 distinct clonal population of MCF-7 NIS expressing cells, 1 with evident membranous NIS staining and the another with predominantly cytoplasmic NIS staining. *In vitro* and *in vivo* studies with radioiodine therapy (^{131}I) in these models showed significant loss in live cell population as compared to control. For in vivo study, the bio-distribution of radioiodine was analyzed by performing *in vivo* Cerenkov Luminescence Imaging (CLI). Radioiodine mediated damage to the NIS expressing tumour cells was observed by performing *in vivo* bioluminescence imaging.Therapeutic potential of NIS in BC is often limited due to low uptake and fast efflux rate of iodine, the scope of using two radio sensitizers i.e. 2-DG and metformin to further improve NIS mediated ^{131}I therapeutic efficacy was explored. Treatment of NIS expressing cells with ^{131}I showed further reduction in cell viability by the application of these radio sensitizers in combination. Our data provides important insights in to the role of NIS as a target gene for treatment of breast cancer.

Publications

Journal

1. Chatterjee S., Malhotra R, Varghese F, et al. Quantitative immunohistochemical analysis reveals association between sodium iodide symporter and estrogen receptor expression in breast cancer. *PloS one.* 2013;8(1):e54055.

2. Chatterjee S., Thaker N., De A. Combined 2-Deoxy Glucose and metformin improves therapeutic efficacy of sodium iodide symporter mediated targeted radioiodine therapy in breast cancer cells. *Breast cancer: targets and therapy (Dove Med Press). 2015;7:251-265*

Other Publications:

1. Chatterjee S., De A. Applications of lentiviral vectors in molecular imaging. Frontiers in Bioscience (Landmark Ed). 2014;19:835-853.

2. Shete H., Chatterjee S., De A., Patravale V. Long chain lipid based tamoxifen NLC. Part II: pharmacokinetic, biodistribution and in vitro anticancer efficacy studies. International journal of pharmaceutics. Sep 15 2013;454(1):584-592.

3. Chatterjee S., Rao V. L. Papineni : Focus on a recent molecular imaging workshop in India. Translational Cancer Research, Vol.2 No. 5, Feb 2013

Conferences

1. Evaluation of Human Sodium Iodide Symporter Gene Expression in Indian breast cancer Subtypes: Sushmita Chatterjee, Frency Varghese, Renu Malhotra, Asawari Patil, Sudeep Gupta and Abhijit De. IACR Annual Meeting, ACTREC, 2012.

2. Combined 2-Deoxy Glucose and Metformin improves therapeutic efficacy of radioiodine treatment in sodium iodide symporter expressing breast cancer cells: Sushmita Chatterjee, Asawari Patil, Vani Parmar, Sudeep Gupta and Abhijit De. WIN Symposium, Paris, France 2014.

3. Understanding the regulatory network of sodium iodide symporter protein glycosylation for improved gene targeted radioiodine therapy : Sushmita Chatterjee, Madhura Kelkar, Shruti B. Menon, Rajiv Kalraiya and Abhijit De. AICBC, CDRI Lucknow 2014.

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11. Name : **Indrajit Sahu**
Enrolment No. : LIFE09201004018
Date of Award of degree : 22.04.16
Constituent Institute : Tata Memorial Centre
Title : Elucidating the Functional Significance of Protein Interaction Networks Mediated by 19S Regulatory Particle of Proteasome.

Abstract

Ubiquitin-Proteasome pathway is the major protein degradation pathway in all eukaryotic organisms, where 26S proteasome plays a central role. The regulatory particle of 26S proteasome (RP), also called 19S-subcomplex, regulate the initial protein degradation processes – substrate recognition, binding, unfolding and deubiquitination in a systematic and precise manner. The six ATPases and some of the Non-ATPases subunits of RP directly involve in substrate degradation process. However, there are some other subunits of19S of whichthe structure and functions are largely uncharacterized viz., PSMD9 and PSMD10. In this current study we elucidated the novel involvement of those above mentioned subunits, in two major cellular signaling pathways in mammalian cells. PSMD9, mainly considered as a proteasomal assembly chaperon, is here found to be involved in NF-κB signaling pathway in a way by degrading the major NF-κB-inhibitory molecule – IκBα. In a greater details, we have demonstrated in this study experimentally that, a novel interacting partner of PSMD9- heterogenous ribonucleoprotein A1 (hnRNPA1) act as a linker between

PSMD9 & IκBα for the proteasomal degradation of IκBα. Furthermore, in a mutational analysis we have also deciphered the binding interface of PSMD9 & hnRNPA1 to the residue level. Mechanistically in this degradation process hnRNPA1 act as a shuttle receptor and PSMD9 as a subunit acceptor on proteasome. However, some of the upstream events in this pathway is still unclear and yet has to be elucidated. Nevertheless, here we have provided the first line of evidence for the novel involvement of PSMD9 in NF-κB signaling pathway and speculated the interaction interface between PSMD9-hnRNPA1 as a potential drug target in cancer cells. PSMD10, a non-ATPase of 19S-RP, also known as gankyrin, is a well established oncoprotein and involved in many cancers. In this current study we took an attempt to elucidate its normal functions in our in vitro model system – Neural progenitor cells. From our preliminary data we found PSMD10 as a potent modulator for neuronal differentiation process. However, the molecular pathways modulated by PSMD10 during this differentiation process has to deciphered in future which may lead to develop a new treatment modality for neuronal disorders.

Publications

Journal

1. Sahu I, Sangith N, Ramteke M, Gadre R, Venkatrama P. (2014). A novel role for the proteasomal chaperone PSMD9 and hnRNPA1 in enhancing IκBα degradation and NF-κB activation – functional relevance of predicted PDZ domain–motif interaction. *FEBS J*. Vol. 281 (11), 2688-2709.

2. Sangith N, Srinivasaraghavan K, Sahu I, Desai A, Medipally S, Somavarappu A. K, Verma C, Venkatraman P. (2014). Discovery of novel interacting partners of PSMD9, a proteasomal chaperone: Role of an Atypical and versatile PDZ-domain motif interaction and identification of putative functional modules. *FEBS Openbio*. Vol 4, 571–583.

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12. Name : **Bonu Venkataramana**
Enrolment No. : PHYS02201004002
Date of Award of degree : 18.04.16
Constituent Institute : Indira Gandhi Centre for Atomic Research
Title : Growth and Physico-chemical Properties of .
Semiconducting SnO2 Nanostructures

Abstract

The wide usage of SnO_2 nanostructures (NSs) [quantum dots (QDs), nanoparticles (NPs), and nanowires (NWs)] in the areas such as waveguides, solar cells, Li-ion batteries, gas sensing, transparent electrodes, and in electro chemistry made this material technologically important. During my PhD, I have developed expertise in chemical synthesis of SnO_2 NPs of six different sizes starting from 2.4 nm (QDs) to 25 nm. I have also grown three different morphological (cylindrical, square, and belt shaped) SnO_2 NWs by chemical vapor deposition (CVD) system. TEM, FESEM, XRD, and AFM techniques were used to probe morphological and structural properties of the SnO_2 nanostructures. Apart from size of nano crystals the defects in SnO_2 such as 'O' vacancies and surface –OH groups plays crucial role in its applications. Presence and the role of defects in SnO_2 nanostructures were studied with the aid of Raman spectroscopy, tip enhanced Raman spectroscopy (TERS), Photoluminescence, and X-ray photoelectron spectroscopy (XPS). Oxygen vacancy related Photoluminescence of NSs was studied in the temperature range from 80 to 373 K. Pristine approach was taken in revealing –OH groups related defect band and corresponding photoluminescence using low energy excitation. Surface –OH groups caused aqua stability of QDs was studied with respect to time. Conventional micro Raman spectroscopy was explicitly utilized in understanding influence of temperature (80-773 K) on size dependent low frequency Raman modes, defect related modes, and Raman allowed modes of SnO_2.

Expertise on the tip enhanced Raman spectroscopy (TERS) was utilized to probe defect and size dependent modes of SnO_2 NPs at room temperature for the first time on the SnO_2 NPs. Stoichiometry of NPs was probed by XPS. With experience on these techniques, role of defects and size of nanostructures are elucidated and tangible correlations with chemical gas sensing (CH_4, O_2 and H_2), magnetism, and energy absorption spectra of SnO_2 nanostructures were established. Further manipulation of surface properties was also achieved by surface functionalizing SnO_2 NPs with octadecyltrichlorosilanes molecules.

Publications

Journal

1. Invoking forbidden modes in SnO2 nanoparticles using tip enhanced Raman spectroscopy. Venkataramana Bonu, A. Das, S. Dhara and A. K.Tyagi. *J. Raman Spectroscopy* (Rapid Communication), 2015, DOI 10.1002/jrs.4747.

2. Photoluminescence of oxygen vacancies and hydroxyl group surface functionalized SnO2 nanoparticles. Venkataramana Bonu, A. Das, S. Amirthapandian, S. Dhara, and A. K. Tyagi. *Phys. Chem. Chem. Phys*. 2015, 17, 9794-9801.

3. Surface functionalization enhanced magnetism in SnO2 nanoparticles and its correlation to photoluminescence properties. Venkataramana Bonu, A. Das, M. Sardar, S. Dhara, and A. K. Tyagi. *J. Mater. Chem. C,* 2015, 3, 1261-1267.

4. Influence of in-plane and bridging oxygen vacancies of SnO2 nanostructures on CH4 sensing at low operating temperatures. Venkataramana Bonu, A. Das, A. K. Prasad, N. G. Krishna, S, Dhara, and A. K. Tyagi. *Appl. Phys. Lett*. 2014, 105, 243102.

5. Size Distribution of SnO2 Quantum Dots Studied by UV–Visible, Transmission Electron Microscopy and X-Ray Diffraction. Venkataramana Bonu, A. Das. *MAPAN-JMSI*, 2013, 28, 259-262.
6. Synthesis and surface functionalization of SnO2 nanoparticles and their superhydrophobic coatings. Venkataramana Bonu, A. Das, S. Dhara, S. Amirthapandian and A. K. Tyagi. *Sci. Adv. Mater*. 2013, 5, 865-873.

Conference Proceedings

1) Intrinsic high magnetism in SnO2 quantum dots. **Venkataramana Bonu** , A. Das, M. Sardar, S. Dhara and A. K. Tyagi, *AIP Conf. Proc*. **2014**, 1591, 490.

2) Quantum dots SnO2 and Ag/SnO2 for CH4 sensing at low temperature (Oral Presentation) A. Das, **Venkataramana Bonu**, A.K. Prasad, S. Dhara, D.Panda, R. Amala, and A. K. Tyagi, Intl. Union of Mater. Res. Soc.-International Conference in Asia (December 16-20, 2014) Bangalore, India
3) Intrinsic high magnetism in SnO2 quantum dots (Oral Presentation) **Venkataramana Bonu**, A. Das, M. Sardar, S. Dhara and A. K. Tyagi, DAE Solid State Physics Symposium (DAE-SSPS-2013) Patiala, India
4) SERS substrates of Ag nanoparticles for CTAB capped Ag LB films. A. Das, **Venkataraman Bonu**, J. John, S. Dhara, A. K. Tyagi, International Conference on Raman Spectroscopy (ICORS, August 13-17 2012) Bangalore, India.
5) Surface functionalization mediated enhanced magnetic moments in SnO2 NPs. **Venkataramana Bonu** , A. Das, M. Sardar, S. Dhara and A. K. Tyagi, International Conference on Nanoscience and Technology (ICONSAT-2014), Panjab University, Chandigarh, India.

6) Evolution of quantum dots to one-dimensional SnO_2 and its sensing applications.**Venkataramana Bonu** , A. Das, S. Dhara and A. K. Tyagi. Materials Research Society of India (MRSI)- Theme Symposium-2013 on Advanced Materials for Energy Applications, IGCAR, Kalpakkam, India.

7) Onset of Low Temperature CH_4 Sensing in Nanostructured SnO_2. A. Das, **Venkataramana Bonu**, International Conference on Nanoscience and Nanotechnology, SRM University, Chennai, India.

8) SnO_2 Quantum Dots retaining Optical and Electrical Properties in LB films. Das, **Venkataramana Bonu**, V. Jeya Karthika and V. Deepika.

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13. Name : **Arnab Ghosh**
Enrolment No. : PHYS07201004002
Date of Award of degree : 22.04.16
Constituent Institute : Institute of Physics,
Title : Growth, Characterization and Applications of Variable Oxygen Deficient Oxide Hetero-nanostructures (Au-ZnO and Au-GeO2).

Abstract

This thesis work is focused on the growth of two different wide direct band gap oxide semiconductor-metal (Au-ZnO and Au-GeO_2) hetero-nanostructures (HNs) of various morphologies and oxygen defect densities, and their enhanced visible-light driven applications with modified properties. The use of these wide direct bandgap homogeneous (single material component) nanostructures (ZnO and GeO_2) towards visible-light driven applications are hindered by some apparent drawbacks: (i) they only can absorb ultraviolet light ($\lambda <$ 380 nm) and have very limited visible light response; (ii) fast radiative recombination rate of photogenerated electron–hole pairs (e^--h^+ pairs). In this regard it is now paramount to develop standard ways not only to enhance their visible-light absorption capability but also to restrain fast radiative recombination processes for their practical optoelectronic and photocatalytic device applications. In recent past, significant efforts have been devoted to improve visible-light driven activities of wide band gap OS NSs, through a time consuming and multistep chemical or physical processes and hence an expensive processes. In contrast, this thesis work demonstrate a novel *single step* Au catalyzed chemical vapor deposition (CVD) technique to grow various oxygen deficient Au capped ZnO and GeO_2 HNs having efficient visible-light harnessing capabilities as well as prolonged lifetime of photogenerated electron-hole pairs. Possible mechanisms behind the growth of these Au-ZnO and Au-GeO_2 HNs have been proposed and discussed in detail. In addition, several issues, which actively influence the growth of these HNs, (via VLS and/or VS growth mode) such as, role of catalyst and its thickness, substrates type and orientations, native oxide on Si substrate, growth ambiance and vapor pressure have been well addressed. These intrinsically self-assembled Au-ZnO and Au-GeO_2 HNs are further utilized towards multifaceted applications, such as, robust SERS detection of CV molecule, photocatalytic degradation of hazardous organic pollutant under visible-light, electron field emission (FE) with tailored work function and visible-light photodetection. Visible-light driven activities towards above mentioned applications are documented with a detailed mechanism. Enhanced FE properties offered by Au-ZnO HNs has been attributed to the reduction in work function due to the combined presence of oxygen vacancy and Au in them, probed by experiments and qualitatively supported by DFT calculations. In spite of having high bandgap of GeO_2 ($\approx$ 4.8-5.1 eV), the visible-light photodetection application of Au-GeO_2 N/MWs grown in Ar ambiance following their lower reflectance and photoluminescence in the visible regime, has been explored for the first time.

Publications

Journal

1. *Study of Faceted Au nanoparticle capped ZnO nanowires: Antireflection, Surface Enhanced Raman Spectroscopy and Photoluminescence aspects.
   Arnab Ghosh, R. R. Juluri, P. Guha, R. Sathyavathi, A. Dash, B. K. Jena and P. V. Satyam,

   J. Phys. D: Appl. Phys. **48**, 055303 (2015).
2. *Simple growth of faceted Au–ZnO hetero-nanostructures on silicon substrates (Nanowires and Triangular Nanoflakes): A shape and defect driven enhanced photocatalytic performance under visible light.
   Arnab Ghosh, P. Guha, A. K. Samanatara, B. K. Jena, R. Bar, S. K. Ray and P. V. Satyam,

   ACS Appl. Mater. Interfaces **7 (18)**, 9486 (2015).
3. *Tuning work function of randomly oriented ZnO nanostructures by capping with faceted Au nanostructure and oxygen defects: Enhanced field emission experiments and DFT studies.
   Arnab Ghosh, P. Guha, R. Thapa, S. Sinthika, M. Kumar, B. Rakshit, T. Dash, R. Bar, S. K. Ray and P. V. Satyam,

   Nanotechnology **27**, 125701 (2016).
4. *Novel large scale growth of Au-GeO_2 nano/micro-wires: Surface-plasmons and oxygen-defects mediated visible-light photodetection.
   Arnab Ghosh, P. Guha, S. Mukherjee, R. Bar, S. K. Ray and P. V. Satyam,

   To be submitted, 2016.
5. *Role of native oxide on Si substrate towards Au catalyzed growth of ZnO nanowires: Transition of growth mode from VLS to VS or vice versa
   Arnab Ghosh, P. Guha, A. Bhukta and P. V. Satyam,

   Manuscript under preparation.
6. Growth of Ag nanostructures on high-index Si (5 5 12) surfaces under UHV conditions: effect of prior surface treatment before deposition
   A. Bhukta, P. Guha, **Arnab Ghosh**, P. Maiti and P. V. Satyam,

   Appl. Phys. A **122**, 356 (2016).
7. Silver endotaxy in silicon under various ambient conditions and their use as surface enhanced Raman spectroscopy substrates.
   R. R. Juluri, **Arnab Ghosh**, A. Bhukta, R. Sathyavathi and P. V. Satyam,

   Thin Solid Films **586**, 88 (2015).
8. Multilayer Ge Nanocrystals embedded within Al2O3 matrix for high performance floating gate memory devices.
   R. Bar, R. Aluguri, S. Manna, **Arnab Ghosh**, P. V. Satyam and S. K. Ray,

   Appl. Phys. Lett. **107**, 093102 (2015).
9. Sandwiched graphene with nitrogen, sulphur co-doped CQDs: Efficient metal free material for energy storage and conversion application.
   A. K. Samantara, S. C. Sahu, **Arnab Ghosh** and B. K. Jena,

   J. Mater. Chem. A **3**, 16961 (2015).

10. Coherently Embedded Ag Nanostructures in Si: 3D Imaging and their application to SERS.
R. R. Juluri, A. Rath, **Arnab Ghosh**, A. Bhukta, Sathyavathi R., Narayana rao D., K. Mueller, K. Frank, M. Schowalter, T. Grieb, F. Krause, A. Rosenauer and P. V. Satyam,

Sci. Rep.(Nature) **4**, 4663 (2014).

11. Study of initial stages of growth of Au-assisted epitaxial Ge nanowires on clean Ge(100) Surface.
A. Rath, J. K. Dash, R. R. Juluri, **Arnab Ghosh**, T. Grieb, M. Schowalter, F. F. Krause, K. Müller, A. Rosenauer and P. V. Satyam,

CrystEngComm. **16**, 2486 (2014).

12. Facile synthesis of single crystalline n-/p- type ZnO nanorods by lithium substitution and their photoluminescence, electrochemical and photocatalytic properties.

I. Thakur, S. Chatterjee, S. Swain, **Arnab Ghosh**, S. K. Behera and Y. S. Chaudhary,

New J. Chem. **39**, 2612 (2015).

13. Substrate Symmetry Driven Endotaxial Silver Nanostructures by Chemical Vapor Deposition.
R. R. Juluri, A. Rath, **Arnab Ghosh** and P. V. Satyam,

J. Phys. Chem. C **117 (25)**, 13247 (2013).

14. A bioinspired approach for shaping Au nanostructures: The role of biomolecule structures in shape evolution.
S. C. Sahu, A. K. Samantara, **Arnab Ghosh** and B. K. Jena,

Chem. Eur. J. **19**, 8220 (2013).

15. Polarity selective etching: A self-assisted route for fabricating high density of c-axis oriented tapered GaN nanopillars.
Arnab Ghosh, H. P. Bhasker, A. Mukherjee, T. Kundu, B. P. Singh, S. Dhar, S. De and A. Chowdhury,

J. Appl. Phys. **110**, 033528 (2011).

16. Photoluminescence study on irradiated yttria stabilized zirconia.
R. Halder, P. Sengupta, V. Sudarsan, A. Ghosh, **Arnab Ghosh**, A. Bhukta, G. Sharma, I. Samajdar and G. K. Dey,

J. Nucl. Mater. **456**, 359 (2015).

17. Electron irradiation induced buckling, morphological transformation, and inverse Ostwald ripening in nanorod filled inside carbon nanotube.
A. Singh, R. Kumari, V. Kumar, L. Krishnia, Z. Naqvi, A. K Panwar, U. M. Bhatta, **Arnab Ghosh**, P. V. Satyam and P. K. Tyagi,

Appl. Surf. Sci. **360**, 1003 (2016).

18. Good's Buffer Derived Highly Emissive Carbon Quantum Dots: Excellent Biocompatible Anticancer Drug Carrier.
A. K. Samantara, S. Maji, **Arnab Ghosh**, B. Bag, R. Dash and B. K. Jena,

J. Mater. Chem. B (Accepted, 2016).

19. Polysaccharide-capped silver Nanoparticles inhibit biofilm formation and eliminate multi-drug-resistant bacteria by disrupting bacterial cytoskeleton with reduced cytotoxicity towards mammalian cells.
S. Sanyasi, R. K. Majhi, S. Kumar, M. Mishra, **Arnab Ghosh**, M. Suar, P. V. Satyam, H. Mohapatra , L. Goswami and C. Goswami,

Sci. Rep.(Nature) (Revised version submitted, 2016).

Conference Presentations

1. *Single step growth of Au-ZnO hetero-nanostructures and their application as1 efficient cold field Emitter: Experimental study and DFT simulation.
   Arnab Ghosh, P. Guha, R. Thapa, S. Sinthika, M. Kumar, B. Rakshit, T. Dash and P. V. Satyam,

   NANOSA-2015, 24th – 28th August 2015, MPI-PKS, Germany.
2. *Structural characterization of simultaneously grown two types of Au-ZnO hetero-nanostructures (Nanowires and triangular nanoflakes) using electron microscopy.
   Arnab Ghosh, R. R. Juluri, P. Guha, M. Kumar and P.V. Satyam,

   EMSI-2015, 8th – 10th July 2015, Mumbai, India.
3. *Optical, photo-electrochemical and field emission properties of Au-ZnO Nanowires.
   Arnab Ghosh, R. R. Juluri, P. Guha and P. V. Satyam,

   PSI-2014, 24th – 28th February 2014, Puri, India.
4. *Structure and optical properties of 1D ZnO nanostructures on Si substrate.
   Arnab Ghosh, R. R. Juluri and P. V. Satyam,

   EMSI-2013, 3rd – 5th July 2013, Kolkata, India.
5. Role of vacuum level on surface morphological modifications in Au/Si(100) system: An in-situ and ex-situ TEM study.
   A. Rath, J. K. Dash, R. R. Juluri, **Arnab Ghosh** and P. V. Satyam,

   EMSI-2012, 2nd – 4th July 2012, IISc Bangalore, India.
6. Shape Transition in Au/Si (100) System: Role of Surface oxide and Vacuum level.
   A. Rath , J. K. Dash , R. R. Juluri1, **Arnab Ghosh**, A. Rosenauer and P. V. Satyam, *ICANN-2011*, 8th – 10th December 2011, IIT Guwahati, India.

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14. Name : **Lalith Kumar Chaganti**
Enrolment No. : LIFE09200804004
Date of Award of degree : 22.04.16
Constituent Institute : Tata Memorial Centre
Title : Role of HtrA2 and its Domains in Regulating its Specificity and Functions

Abstract

HtrA2 is a trimeric pyramidal proapoptotic serine protease whose expression is altered in ovarian, gastric, prostate and breast cancers. It is involved in mitochondrial homeostasis and induction of apoptosis through caspase-dependent as well as independent pathways thus making it a potential drug target in cancer therapy. The protein comprises a short N-terminal region, a serine protease domain and a C-terminal PDZ regulatory as well as protein-protein interaction domain. Despite the availability of inactive protease crystal structure, its molecular mechanism and dynamics of action is still elusive. Using structure-guided design, molecular simulation and functional enzymology, we have characterized various combinations of HtrA2 domains and mutants. Further to understand the proapoptotic property of HtrA2, we delineated its interaction with one of its anti-apoptotic binding partner Pea-15. Our findings highlight importance of N-terminal region, oligomerization, and intricate intermolecular PDZ-protease cross talk work in a precise coordinated fashion towards formation of a catalytically competent HtrA2. Interaction studies with Pea15 provide first mechanistic insight into the substrate recognition and specificity of HtrA2. Binding studies with

Pea15 define a bipartite mode of interaction between HtrA2 and Pea15. Enzymology results suggest that allosteric activation of HtrA2 might be required by adaptor proteins in the cell to relieve the inhibitory effect of PDZ domain. Substrate specificity analyses reveal that HtrA2 has broad selectivity toward the residues neighboring the cleavage-site.Our advancement in understanding toward HtrA2 mechanism of action will help in developing tailored allosteric effectors that enhances the proteolytic activity of HtrA2 towards its substrates. This could be a promising therapeutic strategy against the varied diseases associated with it.

Publications

Journal

1. Intricate structural coordination and domain plasticity regulate activity of serine protease HtrA2. Chaganti LK, Kuppili RR, Bose K. FASEB J 2013; 27(8):3054-66

2. Allosteric regulation of serine protease HtrA2 through novel non-canonical substrate binding pocket. Bejugam PR, Kuppili RR, Singh N, Gadewal N, Chaganti LK, Sastry GM, Bose K. PLoS ONE 2013;8(2):e55416. doi: 10.1371

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1. Cathepsins and HtrAs – Multitasking Proteases in Programmed Cell Death. In Proteases in Apoptosis: Pathways, Protocols and Translational Advances. Chaganti LK, Singh N, Bose K. Ed. Kakoli Bose. Switzerland. Springer International Publishing, 2015. 95-141
2. Proteases in Apoptosis: Protocols and Methods. In Proteases in Apoptosis: Pathways, Protocols and Translational Advances. Acharya S, Kuppili RR, Chaganti LK, Bose K. Ed. Kakoli Bose. Switzerland. Springer International Publishing, 2015. 143-202.

Conferences

1. Presented poster entitled "Role of structural plasticity and inter domain contacts in regulating HtrA2 function" by 31st annual convention Indian association of cancer research and international symposium in cancer genomics and its impact in the clinics. Organized by Advanced Centre for Treatment Research and Education in Cancer, Tata Memorial Centre, Kharghar, Navi-Mumbai, and Maharashtra, India. January 26-29, 2012
2. Presented poster in National Symposium on "FRONTIERS OF BIOPHYSICS, BIOTECHNOLOGY & BIOINFORMATICS" & 37th ANNUAL MEETING OF INDIAN BIOPHYSICAL SOCIETY (IBS).Organized by Department of Biophysics & Centre for Excellence in Basic Sciences, University Of Mumbai, Mumbai. January 13-16, 2013
3. Presented poster in International Symposium on Conceptual Advances in Cellular Homeostasis Regulated by Proteases and Chaperones the Present, the Future and Impact on Human Diseases. Organized by Advanced Centre for Treatment Research and Education in Cancer, Tata Memorial Centre, Kharghar, Navi-Mumbai, and Maharashtra, India. December 3-6, 2013

4. Presented poster at biophysics-pashchim V meeting organized by Tata Institute of Fundamental Research, Mumbai, India
5. Presented poster and a short talk in biophysics-pashchim VI meeting organized by IISER, Pune, India

15. Name : **Mohini Guleria**
Enrolment No. : CHEM01201004013
Date of Award of degree : 27.04.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Development Of Diagnostic And Therapeutic Radiotracers For Targeting Tumors Using Different Approaches.

Abstract

The work carried out in present thesis describes the preparation of different radiolabeled agents for use as targeted radiotracers, in different applications and their preliminary bioevaluation in suitable animal models. Biomolecules which were utilized in the present study include porphyrin derivatives, monoclonal antibodies, peptide and nitroimidazoles. Each of these biomolecules is used for targeting tumor lesions by use of independent and unique mechanism. The aim of this work was to design specific radiotracers for different tumors making use of different carrier molecules as targeted vectors and also to demonstrate their tumor targeting abilities in diagnostic or therapeutic applications. This thesis has been divided into four chapters.Chapter one gives a brief overview of radiopharmaceuticals and their usage in nuclear medicine. General methods of production of radioisotopes with their merits and inadequacies for a particular application are described with an emphasis on the generator-produced radioisotopes (^{99m}Tc, ^{68}Ga and ^{90}Y) and reactor produced isotope (^{177}Lu). Chapter two describes the use of porphyrins in designing radiolabeled agents for targeting tumor, the mechanisms involved, details of syntheses of different derivatives of porphyrin, their radiolabeling with suitable radionuclides (^{68}Ga, ^{177}Lu and ^{90}Y) and preliminary evaluations in suitable animal tumor models. In Chapter three, targeting receptor over expression in specific tumors, using two different types of molecular vectors such as monoclonal antibodies (mAbs) and RGD peptide is discussed. Chapter four describes the preparation of neutral ^{99m}Tc(CO)$_3$-complexes of 2-, 4-, and 5-nitroimidazole derivatives for imaging of tumor hypoxia. The complexes were subsequently evaluated in Swiss mice bearing fibrosarcoma tumor.

Publications

Journal

1. Synthesis and bio-evaluation of a ^{177}Lu-labeled unsymmetrical cationic porphyrin derivative as a tumor targeting agent. **Mohini Guleria**, Tapas Das, Haladhar Dev Sarma, Sharmila Banerjee. *Journal of Radioanalytical and Nuclear Chemistry,* 307, 1537-1544 **(2016).**
2. Neutral ^{99m}Tc(CO)$_3$ complexes of "clicked" nitroimidazoles for the detection of tumor hypoxia. **Mohini Bhadwal**, Madhava B Mallia, Haladhar Dev Sarma, Sharmila Banerjee. *Journal of Radioanalytical and Nuclear Chemistry*, 307, 69-77 (**2016**).
3. Radiosynthesis and bioevaluation of ^{68}Ga-labeled 5,10,15,20-tetra(4-methylpyridyl)-porphyrin for possible application as a PET Radiotracer for tumor imaging. **Mohini Bhadwal**, Tapas Das, Haladhar Dev Sarma, Sharmila Banerjee. *Molecular Imaging and Biology*, 17, 111-118 (**2015**).
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2. Preparation and preliminary in vitro evaluation of ^{177}Lu-labeled Rituximab; Sweety Mittal, **Mohini Bhadwal**, Chandan kumar, Tapas Das, Grace Samuel, M.R.A. Pillai; *World Journal of Nuclear Med*icine, 12, 88-89 (**2013**).
3. Neutral ^{99m}Tc(CO)$_3$ complexes of "clicked" nitroimidazoles for the detection of tumor hypoxia; **Mohini Bhadwal**, Madhava B Mallia, Haladhar Dev Sarma, Sharmila Banerjee; *Indian Journal of Nuclear Medicine*, 28, S46 (Abstract), (**2013**).

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16. Name : **P. Akhilesh**
Enrolment No. : MATH08200904003
Date of Award of degree : 27.04.16
Constituent Institute : Harish-Chandra Research Institute
Title : Chromatic Sums Of Squares And Primes.

Abstract

For any integer K that is at least 1, let s(K) be the smallest integer such that when squares of the natural numbers are each coloured in one of K colours, every sufficiently large integer can be written as a sum of at most s(K) squares, all of the same colour. Also, let t(K) be the corresponding integer in the analogous context for the set of primes. A problem proposed by A. Sárközy asks for optimal bounds for s(K) and t(K) in terms of K. The main result in this thesis is an upper bound for s(K) that improved on the best known upper bound for s(K). This is obtained in Chapter 2 of the thesis. Chapter 3 of the thesis gives a simplified proof for the essentially optimal upper bound for t(K). A key tool in these chapters is the large sieve inequality and certain analogues of it. Chapter 4 of this thesis, which is its final chapter, concerns the Beurling-Selberg function. This function has a number of applications in analytic number theory, in particular to the large sieve inequality. In the final chapter we give an essentially complete account of the standard properties of the Beurling-Selberg functionby viewing it as a solution to a difference equation.

Publications

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1. "A Remark on the Beurling-Selbergfunction", P. Akhilesh and D.S. Ramana, Acta Math. Hungarica, **2013**, 139 no. 4, 354-362.
2. "A Chromatic version of Lagrange's Four Squares Theorem", P. Akhilesh and D.S. Ramana, MonatsheftefürMathematik, **2015,** 176 no. 1, 17-29.

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17. Name : **Nagaraj Alangi**
Enrolment No. : ENGG01200704009
Date of Award of degree : 27.04.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Development of molten salt electrochemical process for electrolytic reduction of uranium oxide.

Abstract

Electrolytic reduction of uranium oxide for producing uranium metal has assumed importance because of the introduction of metallic fuels and atomic vapour laser isotope separation (AVLIS) in the nuclear fuel cycle. Conventionally, UF_4 containing electrolytes are used in the electrolytic reduction of uranium oxide, which pose problem in tailoring the solvent for specific isotopic composition of uranium. LaF_3 is proposed as an alternative solvent for UF_4 in the electrolytic reduction of uranium oxide. TG-DTA and X-Ray Diffraction studies were done on several salt mixtures to determine the melting points, high temperature losses due to evaporation and room temperature phases present. A detailed conditioning procedure was developed with Linear sweep voltammetry diagnostics. Selection of materials to handle fluoride baths had been done based on thermodynamic analysis and experiments simulating the electrolysis process. The solubility of UO_2 in the molten mixtures of equimolar LiF-BaF_2(1:1) with LaF_3 as additive was studied in the range of 1423K to 1523K. Studies were conducted in the range of 10% to 50% by weight additions of LaF_3 in the equimolar LiF-BaF_2(1:1) base fluoride salt bath. Solubility of UO_2 increased with rise in LaF_3 concentration in the molten fluoride in the temperature range of 1423K-1523K. At a given concentration of LaF_3, the UO_2 solubility increased monotonously with temperature. With mixed solvent, when UF_4 was added as a replacement of part of LaF_3 in LiF-BaF_2(1:1)-10 wt% LaF_3 and LiF-BaF_2(1:1)-30 wt% LaF_3, there was an enhancement of solubility of UO_2.Electrochemical studies on UF_4 or LaF_3 in LiF-BaF_2 eutectic were carried out with and without UO_2 at 1473K by cyclic voltammetry and chronopotentiometry. In the electrolyte LiF-BaF_2 (1:1)25 wt% UF_4 the measured reduction potentials of $U^{4+} \rightarrow U^{3+}$ and $U^{3+} \rightarrow U$ are -0.804V and -0.999V respectively versus platinum quasi reference electrode (QRE) at 1473K. It was observed that cathodic peak potentials shifted more cathodically with increase in scan rate, indicating a quasi-reversible reduction process. Chronopotentiograms exhibited waves corresponding to voltammogram peaks and have been found to follow the Sand's law. With the addition of UO_2 to the LiF-BaF_2(1:1)-25 wt% UF_4 / LaF_3 electrolyte, only a broad peak appears indicating that uranium may be present as an oxy-fluoride complex. Electrolytic reduction experiments were conducted and the effects of the following were studied: a) Variation of the size of the cell, b) anode and cathode configurations, c) cathode or liquid cathode materials, d) anode materials and e) type of electrolytes. Several electrolysis experiments were conducted in LiF:BaF_2 (1:1)-25 Wt % UF_4 salt mixtures to arrive at the cell configuration. Thereafter, the experiments were continued for production of uranium in the electrolytes proposed in the study. The electrolysis experiments with ~60g tin or copper as the liquid cathode in BN container and UO_2 as anode with ~1400g of electrolyte with a current density of ~2 A/cm^2 yielded mixture of Tin-USn_3 and Cu-Cu_5U, respectively; this confirmed the formation of uranium metal. Process repeatability in LiF:BaF_2:25%LaF_3 electrolyte was established. ~8% cathode current efficiency was observed in LiF:BaF_2:25% LaF_3 electrolyte.A systematic and comprehensive study is reported for the preparation of robust yttria coatings on components. A series of coating experiments were conducted by producing the coatings of yttria with variation of powder size, plasma power, primary glass flow and powder feed rate. Adhesion test was used as the response parameter for obtaining the optimum coating parameters. The coatings produced did not develop any cracks upto 26 cycles during thermal cycling. Compatibility of the coated coupons with liquid uranium was studied by immersing the coated coupons into liquid uranium at 1573K for different durations. Separate experiments were conducted by continuous immersion for 10, 20, 40, 80, 120, 200 and 400hrs durations. The cross-sectional micrograph had shown that the coating is relatively free of interconnected pores. None of the coupons showed delamination or interfacial cracks. No specific reaction products were observed at the liquid/Y_2O_3 interface in all the coupons.

Non-stoichiometric yttrium oxide was not observed across the thickness of coating even after 400 hrs of contact time with liquid uranium.

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Journal

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2. Nagaraj Alangi, Jaya Mukherjee, L M Gantayet, "Electrochemical study of uranium in molten fluoride media at 1473K", to be communicated to Journal of applied electrochemistry.

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1. Nagaraj A., Anupama P., Jaya Mukherjee, K. P. Sreekumar, R. U. Satpute, P. V. A. Padmanabhan, L. M. Gantayet, "Studies on thermal stability of plasma sprayed yttrium oxide coatings deposited on pure tantalum substrate", NMD-ATM 2007.
2. Nagaraj A, Trupty Chavan, D.N.Wagh, Anupama P., R.Verma, L.M.Gantayet, "Determination of Uranium in molten fluoride salts using Energy Dispersive X-ray fluorescence (EDXRF)", NUCAR 2009.
3. Nagaraj Alangi, Jaya Mukherjee, Anupama P, M K Verma, Y Chakravarthy, "Thermal and chemical stability studies of protective plasma sprayed yttrium oxide coatings on tantalum substrate against liquid uranium“, International Conference on Electron Nanoscopy, EMSI50, 2011.
4. Nagaraj Alangi, Anupama P., Jaya Mukherjee, L. M. Gantayet, "Evaluation of a molten salt electrolyte for direct reduction of actinides", Advances in Nuclear Materials, ANM- 2011.
5. Nagaraj Alangi, A K Suri and L M Gantayet, " Electrochemical study of uranium in molten fluoride media at 1473K", NuMat 2012: The Nuclear Materials Conference, Osaka, Japan, 22-25 October, 2012.
6. Nagaraj Alangi, Jaya Mukherjee, Anupama P, K Dasgupta, "Electrolytic reduction of ranium oxide in molten fluoride baths", Thorium energy conference, ThEC2015, Dec 2015.

18. Name : **Sadhan Bijoy Deb**
Enrolment No. : CHEM01200804010
Date of Award of degree : 27.04.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Synthesis, Characterization And Coordination Chemistry Of Hard And Soft Donor Ligands With Lanthanides And Actinides.

Abstract

Incinerable *iso*-butyramide based ligand were synthesized and their complexing behavior towards the uranyl, thorium, lanthanum nitrates and uranyl *bis* (β-diketonates) were studied to see the feasibility for using these ligands for the selective separation of uranium by precipitation method instead of solvent extraction process, thereby reducing the number of steps involved during separation process. Systematic structural studies on *iso*-butyramide uranyl complexes were evaluated . The stability and selectivity for these ligands towards uranyl ion can be explained on the basis of strong bonding between the amide oxygen and uranyl group. The observed bond distances between the uranium and oxygen atom of amide group [~ 2.35 Å] are much short in lengths as compared to those of other reported U-O(amide) bond distances and comparable to those of U-O(phosphine oxide) distances. The synthesis and complexation studies of bis (N, N'-Di-alkyl carbomyl methyl) sulfide, sulfoxide and sulfone based ligands with uranyl and lanthanide ions were also carried out. The structural studies revealed that the thio-diglycolamide ligands bond to uranyl and lanthanum nitrates in a bidentate chelating fashion through the carbamoyl oxygen atoms and the thio-ether group is un-coordinated. These structures are very similar to that of the uranyl nitrate–malonamide compounds. The coordination number around uranium (VI) is eight and the geometry is hexagonal bi-pyramidal whereas , for lanthanum (III) it is ten and the geometry is a distorted bi-capped square-anti-prism. The NMR spectra reveal that the thioglycolamide ligands are weakly bonded to the lanthanum nitrate in solution. The structure of *bis* (carbamoyl methyl) sulfoxide, uranyl nitrate shows that the ligand bonds to metal ion in a bidentate chelating fashion through the carbamoyl and sulfoxo oxygen atoms. It shows further that one of the carbamoyl oxygen atoms is uncoordinated. The coordination number around uranium (VI) is eight and the geometry is hexagonal bipyramid. The structure bis (carbamoylmethyl) sulfone, uranyl nitrate shows that the bis (carbamoylmethyl) sulfone ligand bonds to uranyl nitrate in a bidentate chelating fashion through both the carbamoyl oxygen atoms. It shows further that the sulfone group is uncoordinated. This may be due to the fact that the sulfone group is a poor donor towards the metal centre compared to that of the amide group and therefore the coordination of both the carbamoyl groups to the uranyl ion is observed. The coordination number around uranium (VI) is eight and the geometry is hexagonal bipyramidal. Thermal studies on all complexes show that the ligands are completely incinerable. The sulfoxide and sulfone ligands show no reactivity with the lanthanides under the conditions studied.The phosphine oxide group is well known for its strong complexing ability towards the lanthanide and actinide ions. The synthesis and structural studies of bis (diphenylphosphine oxide) ferrocene with uranyl nitrate and uranyl dichloride were carried out. These compounds were characterized by CHN analysis, IR, NMR and XRD techniques. The molecular structure of [$UO_2(NO_3)_2DPPFO_2$] shows that the uranium atom is surrounded by eight oxygen atoms in a hexagonal bi-pyramidal geometry. The four oxygen atoms of nitrate groups and two oxygen atoms of $DPPFO_2$ form a planar hexagon. The ligand acts as a bidentate chelating ligand and bonds

through both the phosphine oxide oxygen atoms to uranyl group. It is interesting to note that the bite angle between the two P(O) oxygen atoms is 71.56° and is much smaller in value compared to any of the $DPPFO_2$ metal complexes reported so far. The molecular structure of $[UO_2Cl_2\ DPPFO_2]$ shows that the ligands binds to uranium in a bidentate chelating mode and uranium (VI) ion is surrounded by four oxygen and two chlorine atoms in an octahedral geometry. The two chlorine atoms and two oxygen atoms of the $DPPFO_2$ ligand form the equatorial square plane. The U-Cl bond distance 2.634 Å is comparable in magnitude with those of earlier reported uranyl dihalide compounds. The bite angle between the two P(O) oxygen atoms is 82.90°. The chlorides are mutually cis with a Cl-U-Cl angle of 97.75°.

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2. Uranyl(VI) and lanthanum(III) thio-diglycolamides complexes: Synthesis and structural studies involving nitrate complexation. Deb, S. B.; J Gamare, J. S.; S Kannan, S.; Drew, M.G.B., Polyhedron 28 (2009) 2673–2678
3. Synthesis, characterization and molecular structure of 1,1’ bis (diphenyl phosphine Ferrocene) dioxide complex of uranyl nitrate.
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4. Synthesis and structural studies of a bis(carbamoyl methyl) sulfoxide complex of uranyl nitrate.
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6. Synthesis, characterization and molecular structure of 1,1’ bis (diphenyl phosphine ferrocene) dioxide complex of cis-uranyl dichloride.
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2. Synthesis and Structural studies of Bis(Carbomyl Methyl) Sulfone Complex of Uranyl nitrate
   S.Kannan, S.B.Deb and M.G.B.Drew Preprint Vol. of Nuclear and Radiochemistry, held at Gitam University, Visakhapatnam during Feb 22-26 (2011) Paper No. B-33, pp 238-239

19. Name : **V. Mahendran**
Enrolment No. : PHYS02201004010
Date of Award of degree : 27.04.16
Constituent Institute : Indira Gandhi Centre for Atomic Research
Title : Direct Measurements of Colloidal Interactions in the Presence of Analytes.

Abstract

The phase behavior of magnetic nanoemulsions is of considerable research interest from fundamental understanding and application point of view. Besides, magnetic colloidal dispersions are wonderful model systems to probe fundamental issues in condensed matter physics. Understanding of forces between emulsion droplets is essential, in industrial process, materials engineering and biology, to extend the shelf life of formulations. Among various available direct force measurement tools, magnetic chaining technique (MCT) is a unique in-situ force measurement approach that allows measurement of force between magnetic colloidal particles in liquids. The prime objective of this thesis is to get better insights into the effect of cations of various valencies, biomolecules and alcohol molecules on electrostatic and steric forces and the stability of emulsions, such an understanding can aid in the development of ionic and molecular recognition sensors for practical applications. Cation interactions on O/W emulsions lead to a large blue shift in the diffracted wavelength, due to changes in the interdroplet spacing and the electrical double layer around them. The order of increasing of Bragg peak shift for different cations followed a sequence $Pb^{2+} < Ni^{2+} < K^+ < Cu^{2+} < Mn^{2+} < Na^+ < Cd^{2+} < Ca^{2+} < Ag^+$. In the presence of interfering cations, excellent selectivity is observed for Ag^+ due to strong interaction of hydrated Ag^+ with surfactant/polymer. The measurement of intermolecular forces in the presence of alcohol molecules shows that the diffusion of organic molecules into the electric double layer reduces the dielectric constant, resulting in an extended electric double layer and a red shift in the diffracted Bragg peak. The equilibrium interdroplet distance between the emulsion droplets is increased by several nanometers in the presence of glucose because of the intermolecular hydrogen bonding of glucose molecules with SDS molecules. Using the optical response stimulus properties of nanoemulsion, a new methodology to detect MFL signals to image morphologies of defects buried inside ferromagnetic components is developed. Studies on forces between polymer covered emulsion in the presence of casein shows that extended polymer coils are replaced by smaller size casein molecules. On increasing cation concentrations, the adsorbed polymer chains undergo a collapsed conformation. The order of collapse of polymers follows as $Fe^{3+} > Ca^{2+} > Na^+$. The results suggest that the hydrated cations and their interaction with polymer can greatly alter the polymer conformation at oil-water interfaces.

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Journal

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2. "Non-enzymatic glucose detection using magnetic nanoemulsions", V. Mahendran and John Philip, *Appl. Phys. Lett*., 2014,105, 12311.
3. "Influence of Ag^+ interaction on 1D droplet array spacing and the repulsive force between stimuli-responsive nanoemulsion droplets", V. Mahendran and John Philip *Langmuir,* 2014, 30, 10213−10220.
4. "Magnetic nanofluid based approach for imaging defects" V. Mahendran, R. Ancy Beautlin and John Philip, *J. Nanofluids,* 2013, *2*, 165-174.

5. "A Simple, In-Expensive and Ultrasensitive Magnetic Nanofluid Based Sensor for Detection of Cations, Ethanol and Ammonia", J. Philip, V. Mahendran, and Leona J. Felicia, *J. Nanofluids*, 2013, *2*,112-119.
6. "A methanol sensor based on stimulus-responsive magnetic nanoemulsions", V. Mahendran and John Philip, *Sens. Actuators B Chem.*, 2013, *185*, 488–495.
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8. "Spectral response of magnetic nanofluid to toxic cations", V. Mahendran and John Philip, *Appl. Phys. Lett.*, 2013*,102*,163109.
9. "Naked eye visualization of defects in ferromagnetic materials and components", V. Mahendran and John Philip, *NDT & E Int.* 2013, *60*,100 - 109.
10. "An optical technique for fast and ultrasensitive detection of ammonia using magnetic nanofluids", V. Mahendran and John Philip, *Appl. Phys. Lett.,* 2013,*102*, 063107.
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3. V. Mahendran and John Philip "A new method for Detection of Methanol using Magnetic Nanoemulsions" at the *International Conference on Nanoscience and Technology (ICONSAT)-2014* Organized by Institute of Nano Science and Technology, Chandigarh, India during 3-5March, 2014.
4. V. Mahendran and John Philip "Probing of Intermolecular Forces at Interfaces in Presence of Triblock Polymers" at the *13th International Conference on Magnetic Fluids- ICMF-13* held at National Physical Laboratory, New Delhi, India during 7-11 January, 2013. P-365.
5. V. Mahendran and John Philip "Nanofluid based optical sensor for detection of defects" at *International Conference on Material Science and Technology (ICMST) -2012*, Kottayam, Kerala, India, during 10-14 June 2012. P-175.

20. Name : **Nitali Dash**
Enrolment No. : PHYS01200804028
Date of Award of degree : 27.04.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Feasibility Studies For The Detection Of Exotic Particles Using Ical At Ino.

Abstract

The 51kton Iron CALorimeter (ICAL) detector at the underground India-based Neutrino Observatory (INO), aims to make a precision measurement of neutrino parameters using atmospheric muon neutrinos (ν_μ's). The dimensions of the ICAL detector are 48 m (length), 16 m (width) and 15 m (height). The tracking nature and comparatively large size of ICAL will allow it to explore new physics in addition to neutrino properties. The thesis is focused on the feasibility studies of physics beyond the Standard Model such as dark matter particles (DMPs) and magnetic monopoles (MMs) using the ICAL. We have looked at a possible search for DM through its decay. The lower limit on the life time of DMP is obtained in INO by considering the decay channel of DMP to lepton (e, μ, τ) pairs. It will not only put the limit on the life time of DMP, it will also clarify the observation of the anomalous Kolar events recorded in the 70's and 80's by experiments at Kolar Gold Field (KGF). These have been reinterpreted as due to the decay of dark matter particles recently. In the second aspect, as ICAL is a tracking detector, there is the possibility of detecting MM in the sub-relativistic region. These are characterised by the large time intervals from 0.5ns up to 0.3 μs, corresponding to β of 0.7 to 10^{-3} between the signals in successive layers of the RPC detectors. The sensitivity of ICAL is found to be sensitive to the MMs in the mass range from $10^{7} - 10^{17}$GeV with β ranging from $10^{-3} - 0.7$.

Publications

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3. A Study on the time resolution of Glass RPC, N. Dash, V.M. Datar and G. Majumder,arXiv:1410.5532 (2014).

21. Name : **Vinay Jain**
Enrolment No. : LIFE01201004001
Date of Award of degree : 27.04.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Feasibility Studies For The Detection Of Exotic Particles Using Ical At Ino.

Abstract

Human beings are continuously exposed to low levels of ionizing radiation (IR) through various man-made and natural sources. Natural radiation exposures are mainly from terrestrial and cosmic sources whereas man-made low level exposure varies from medical exposures (diagnostic and therapeutic) to accidental exposures such as Chernobyl and Fukushima Daiichi nuclear disasters. Understanding the biological and health effects low dose IR has important implications to human health and radiation protection science. High level natural radiation areas (HLNRA) of Kerala coast provide unique opportunity to study the effect of low dose/dose rate radiation directly on humans. The present thesis emphasized the importance of biological effects of acute and chronic IR and its implication in monitoring of human population. The cellular responses of chronic low level IR have been explored using high throughput techniques to detect changes at low dose exposures. Quantification of DNA double strand breaks (DSBs) was carried using gamma-H2AX biomarker. Transcriptome analysis was carried out to find out differentially expressed genes in HLNRA individuals and detailed bioinformatic analysis was carried out to find out over-represented biological processes and molecular pathways in HLNRA population. Low dose radiation induced conformational changes in chromatin structure was also carried out at acute doses. The thesis revealed some important findings. A marginal reduction in basal level frequency of DNA DSBs was observed in HLNRA individuals (> 5.0 mGy/y) as compared to NLNRA. Interestingly, a background dose dependent increase in the number of differentially expressed genes was observed in HLNRA individuals. An over-representation of DNA repair, DNA damage response, cell cycle regulation, immune response, chromatin/ histone modification and methylation genes was observed in HLNRA individuals (>5.0 mGy/y) indicating active cellular processes occurring in response to chronic low dose radiation in human cells. Radiation responsive genes have been identified which can serve as chronic radiation signatures. The data on DNA damage and transcriptome profile also indicate *in vivo* radio-adaptation of HLNRA individuals in response to chronic low dose exposure. Dynamic Light Scattering (DLS) technique was employed in studying the radiation induced conformational changes in chromatin structure at low dose exposures. The findings of this thesis are highly relevant and beneficial to the scientific community, especially in the field of radiation biology.

Publications

Journal

1. Lack of increased DNA double strand breaks in peripheral blood mononuclear cells of individuals from high level natural radiation areas of Kerala coast in India (2016). Vinay Jain, P.R.Vivek Kumar, P.K.M. Koya, G. Jaikrishan and Birajalaxmi Das. Mutation Research, Fundamental and Molecular Mechanisms of Mutagenesis. http://dx.doi.org/10.1016/j.mrfmmm.2016.03.002 (in press).

2. Radiation induced conformational changes in chromatin structure in resting human peripheral blood mononuclear cells (2014). Vinay Jain, P.A Hassan and Birajalaxmi Das. International Journal of Radiation Biology, 90 (12): 1143-1151.

3. Transcription profile of DNA damage response genes at G_0 lymphocytes exposed to gamma radiation (2012). Divyalakshmi Saini, Shridevi Shelke, A. Mani Vannan, Sneh Toprani, Vinay Jain, Birajalaxmi Das, M.Seshadri. Molecular and Cellular Biochemistry, 364: 271-281.

4. Transcriptional expression of H2B, CTP synthase & PLK3 genes in whole blood exposed to ^{60}Cogamma radiation (2011). Vinay Jain, Birajalaxmi Das and M Seshadri. International Journal of LowRadiation, 8 (1): 55-65.

5. Efficient repair of DNA double strand breaks in individuals from high level natural radiation areas of Kerala coast, south-west India. Vinay Jain, Divyalakshmi Saini, P. R. Vivek Kumar, G. Jaikrishan and Birajalaxmi Das. Scientific Reports (under revision).

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22. Name : **Khageswar Sahu**
Enrolment No. : LIFE03200904002
Date of Award of degree : 29.04.16
Constituent Institute : Raja Ramanna Centre for Advanced Technology,
Title : Applications Of Photodynamic Effects In Dermatology

Abstract

The thesis submitted by Mr. Khageswar Sahu deals with the studies on healing of wounds by topical antimicrobial photodynamic treatment (APDT) mediated by poly- L-lysin chlorin p6 (pl-cp6). The important contributions made by him include **(i)** Providing evidence that APDT of wounds infected with *P. aeruginosa* in mice not only reduces the bacterial load, but also lowers the hyper inflammatory response caused by infection. **(ii)** pl-cp6 mediated APDT expedites healing in both methicillin resistant *S. aureus* (MRSA) and *P. aeruginosa* infected wounds of mice by attenuating degradation of collagen, enhancing epithelialization, hydroxyproline content and collagen remodeling. **(iii)** Compared to single APDT at high light fluence, multiple APDT at lower fluence shows better healing response in MRSA infected wounds in diabetic mice. This has been shown to be due to reduced damage to host cells which consequently improve antibacterial efficacy and enhance level of antioxidants as well as angiogenic growth factors.

Publications

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1. K. Sahu, M. Sharma, P. Sharma, Y. Verma, K.D. Rao, H. Bansal, A. Dube and P. K. Gupta."Effect of poly-L-lysine-chlorin p6 mediated antimicrobial photodynamic treatment treatment on collagen restoration in bacteria infected wounds." Photomed Laser Surg. 32, 23-29 (2014).
2. K. Sahu, M. Sharma, H. Bansal, A. Dube and P.K. Gupta, "Topical photodynamic treatment with poly-L-lysine chlorin p6 conjugate improves wound healing by reducing hyperinflammatory response in Pseudomonas aeruginosa infected wounds of mice." Lasers Med. Sci. 28, 465-471 (2013).
3. K. Sahu, H. Bansal, C. Mukharjee, M. Sharma and P.K. Gupta, "Atomic force microscopic study on morphological alterations induced by photodynamic action of Toluidine Blue O in Staphylococcus aureus and Escherichia coli." J. Photochem. Photobiol. B 96, 9–16 (2009).
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2. K. Sahu, H. Bansal, M. Sharma, A. Dube and P. K. Gupta. "Antimicrobial photodynamic treatment induced by red light and poly-L- lysin conjugated chlorine p6 leads to enhanced nitrite level and healing in Methicillin resistant Staphylococcus aureus infected wounds of diabetic mice". Presentation in National Laser Symposium 2014, Jan 7-10th , Manipal, Udupi (2014) .
3. K. Sahu, M. Sharma, H. Bansal, A. Dube and P. K. Gupta. "Antimicrobial photodynamic treatment induced oxidative stress reduces inflammatory response in Methicillin resistant Staphylococcus aureus infected wounds in diabetic mice". Presentation in 9th DAE-BRNS Life Science Symposium 2013, Nov 28th- 30th, Bhaba Atomic Research Centre, Mumbai (2013).
4. K. Sahu, M.Sharma, A. Dube and P. K. Gupta "Effect of photodynamic therapy on inflammatory response of Pseudomonas aeruginosa infected wounds". Presentation in FIMSA Advanced course on "Basic and translational immunology", Institute for Defence Studies and Analyses, New Delhi during Mar 18-20th (2012).
5. K. Sahu, M.Sharma, P. Kakani, A. Dube, P. K. Gupta. "Photodynamic treatment induced changes in expression of inflammatory cytokines and growth factors in Pseudomonas aeruginosa infected excisional wounds of mice" Presentation in 5th Annual Meeting of Federation of Immunological Society of Asia and Oceania , Mar 14-17th , New delhi (2012).
6. K. Sahu, Y. Verma, M. Sharma, K.D. Rao, A. Dube, P. K. Gupta "Optical Coherence Tomography for Non-invasive Assessment of Wound Healing Response in Pseudomonas aeruginosa infected excisional wounds subjected to Photodynamic Treatment". Presentation in XXXVI Optical Society of India conference " Frontiers in Optics and photonics 2011", Dec 3-5th,Indian Institute of Technology, New Delhi (2011).
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23. Name : **Biswajit Sarkar**
Enrolment No. : ENGG04200904001
Date of Award of degree : 03.05.16
Constituent Institute : Variable Energy Cyclotron Centre
Title : Localization of Mobile Robots in Indoor Environments Using Laser Range Data

Abstract

A necessary prerequisite for autonomous navigation of a mobile robot is the capabilityof localization. If a map of the environment is available with the robot *a priori*,it will be able to localize itself by matching its perception of the environment with the map. However, the processes of automatic map building and that of localization are closely intertwined. Hence,they are solved concurrently, using methods commonly known as *Simultaneous Localization and Mapping* (SLAM).But, in many real-life applications, it is more appropriate to build a map of the working environment first and then use it for localization, rather than operate the robot in online SLAM mode, which is complex, computation-intensive and less accurate. With the objective of achieving robust and accurate localization of mobile robots equipped with laser range findersin (unmodified) indoor environments,which remain practically invariant over extended periods of time, in the thesis, we propose

- an offline method for building maps of indoor environments by merging line segments extracted from registered laser range scans; and
- a robust and accurate method for localization on such maps based on the Monte Carlo framework.

Line segments are a natural choice in the representation of indoor environments. Maps based on line segments are compact, provide floating-point resolutionand scale well with the environment size. The proposed method has been successful in accurately building maps of large environments from datasets available in the public domain as well as from simulated and real-world data. Experimental results show that maps produced by the proposed method are generally better than those produced by two other methods reported in the literature in terms of the compactness and accuracy of the maps.Monte Carlo Localization (MCL) is a powerful and popular approach for mobile robot localization. But MCL has seldom been studied in the context of linesegment-based maps. A key step of the approach is the computation of the so called *importance weight* associated with each hypothesized pose or particle.In this thesis, we propose a novel, heuristic-driven approach for the computationof importance weights in MCL on maps represented with line segments, and extensivelystudy its performance in pose tracking. We also compare our method with three othermethods reported in the literature. The comparative study, conducted using bothsimulated and real data, on maps built from real data available in the public domainclearly establish that the proposed method is more accurate, robust and efficient thanthe other methods.In the concluding part of the thesis, we point out several open issues for furtherresearch. In the backdrop of what has been presented in the earlier part of the thesis,we discuss on a probable way to achieve added robustness and accuracy in localizationso as to make the proposed methods of map building and localization more useful andefficacious for deployment in real-life applications

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Publications

Journal

1) “A novel method for computation of importance weights in Monte Carlo localization on line segment-based maps”, Biswajit Sarkar, Surojit Saha and Prabir K. Pal, Robotics and Autonomous Systems, 2015, 74, Part A, 51 – 65.
2) “Building maps of indoor environments by merging line segments extracted from registered laser range scans”, Biswajit Sarkar, Prabir K. Pal and Debranjan Sarkar, Robotics and Autonomous Systems, 2014, 62, 603 – 615.

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4) “An efficient method for near-optimal polygonal optimization based on differential evolution”, Biswajit Sarkar, International Journal of Pattern Recognition and Artificial Intelligence, 2008, 22, 1267 – 1281.
5) “A genetic algorithm-based approach for detection of significant vertices for polygonal approximation of digital curves”, Biswajit Sarkar, Lokendra Kumar Singhand Debranjan Sarkar, International Journal of Image and Graphics, 2004, 4,223 – 239.
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2) “Localization of mobile robots in indoor environments”, Biswajit Sarkar, Tanushyam Bhattacharjee, Prabir K. Pal and Debranjan Sarkar, in: Proceeding of the Seminar on Applications of Computer & Embedded Technology (SACET) – 2009, Kolkata, India, 2009, 73 – 75.

Others

1) “Localization in of mobile robots in indoor environments using laser range data”,Biswajit Sarkar, Doctoral Symposium, 2015 International Conference on Advances in Robotics (AIR – 2015), organized by the Robotics Society of India, Goa, India, July 5, 2015 (Oral presentation).
2) “Building maps of and localization in indoor environments using a laser range finder, Biswajit Sarkar, International Workshop on Autonomous Vehicles andMobile Robots, Indian Institute of Technology Delhi, July 6 – 8, 2014 (Invited talk).

24. Name : **Sudhir Kumar Shukla**
Enrolment No. : LIFE01201104001
Date of Award of degree : 03.05.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Molecular Studies on Biofilm-associated-protein (Bap) in Staphylococcus aureus.

Abstract

Microbial biofilms are omnipresent and confers high resistance to unfavorable conditions, tolerance to antibiotics or other toxic compounds. *Staphylococcus aureus* biofilm formation on human tissues and prosthetic devices is a serious health concern and it has been shown to be the primary cause of persistent infections. This thesis investigates on several aspects of *S. aureus* biofilm formation with specific focus on the role of Biofilm-associated proteins (Bap). Bap and other surface proteins play a distinct role in formation of *S. aureus* biofilms. An introduction to the bacterial biofilms and Bap proteins has been discussed in the first chapter of the thesis. Subsequently, the study started with a detailed *in silico* characterization of Bap proteins and other homologous proteins. Chapter 3 investigates the role of calcium in the biofilm development by *S. aureus* isolates which showed that calcium regulates the architecture and topography of Bap-mediated biofilm formation. In this context, the entire cycle of biofilm formation was studied using confocal laser scanning microscopy. Chapter 4 investigates the potential use of Proteinase K for dispersal and sensitization of *S. aureus* biofilms for antibiotic treatment where Bap-like surface proteins play a major role in biofilm establishment. In chapter 5, the putative role of c-di-GMP in *S. aureus* biofilm formation/inhibition was investigated. Chapter 6 is an auxillary study where Bap protein was cloned in a suitable vector, overexpressed and purified by Ni-NTA column. The protein was confirmed by SDS-PAGE and Western blotting. Finally, the thesis concludes the findings on *S. aureus* biofilm formation and also focuses on future

Publications

Journal

[1]. Sudhir K. Shukla, T. Subba Rao. Effect of Calcium on *Staphylococcus aureus*biofilm architecture: A Confocal Laser Scanning Microscopic Study. Colloid Surf B: Biointerfaces 2013; 103:448-454.
[2]. Sudhir K. Shukla, T. Subba Rao. Dispersal of Bap-mediated *Staphylococcus aureus* biofilm by proteinase K. The Journal of Antibiotics 02/2013; 66(2):55-60.
[3]. Sudhir K. Shukla, T. Subba Rao. Calcium-Mediated Modulation of Staphylococcal Bacterial Biofilms. Indian Journal of Geo-Marine Sciences 11/2014; 43(11):2107-2116.
[4]. Sudhir K. Shukla, T. Subba Rao. Biofilm removal by targeting biofilm-associated extracellular proteins in bovine mastitis *Staphylococcus aureus* isolates. Indian Journal of Medical Research (accepted).

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[3]. Sudhir K. Shukla, T. Subba Rao. An Improved Crystal Violet Assay for Biofilm Quantification in 96-Well Microtitre Plate. Journal of Microbiological Methods. (Communicated).

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[1]. Sudhir K. Shukla, T. Subba Rao. *Calcium-Mediated Modulation of Staphylococcal Bacterial Biofilms*. International Conference on Advanced Technologies for Management of Ballast Water and Biofouling (MABB- 2014), Chennai, India, 4-7 March 2014.

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[1]. Sudhir K. Shukla, T. Subba Rao. Designing of an anti-biofilm peptide against Bap protein expressing *Staphylococcus aureus* biofilms. International Conference on Medicinal Chemistry, MEDCHEM, 10-11, Sept 2015.
[2]. Sudhir K. Shukla, T. Subba Rao. *Effect of Proteinase K on Staphylococcus aureus Biofilms*. International Conference on Advanced Technologies for Management of Ballast Water and Biofouling (MABB- 2014), Chennai, India, 4-7 March 2014.
[3]. Sudhir K. Shukla, T. Subba Rao. *Antimicrobial activity of N-acetyl cysteine against biofilm forming bacteria*. International Conference on "Microbial World: Recent Innovations and Future Trends", 22-25, November 2012.

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25. Name : **Manoj Kumar Mandal**
Enrolment No. : PHYS08200905003
Date of Award of degree : 06.05.16
Constituent Institute : Harish-Chandra Research Institute
Title : Precise Predictions For Processes Of Interest At Lhc.

Abstract

In this thesis, I have worked mainly in the direction of obtaining precise results for a number of processes at LHC, after incorporating the higher order QCD corrections.I have presented the next-to-leading order QCD predictions for the three photon production in the Standard Model, matched to the parton shower using the MC@NLO formalism in the aMC@NLO framework. Moreover, I have also produced results for di- lepton, di-electroweak boson (ZZ, W+W−) production in both the SM and the ADD model at the NLO+PS accuracy using the same framework, thereby producing a set of realistic events at LHC and making them directly comparable against the experiments. I have studied the role of parton shower on various observables and shown a selection of results for the 8TeV and 14 TeVLHC.In other work, I have mainly worked on the inclusion of the higher order threshold logarithms at higher orders in QCD for the inclusive and semi-inclusive observables for the Higgs boson production. We have provided a framework, based on the factorization properties of the QCD amplitudes along with Sudakovresummation and the renormalization group invariance, that allows one to perform the computation of the threshold corrections in a consistent, systematic and accurate way. Using this framework, we have presented the rapidity distribution of the Higgs boson produced through bottom quark annihilation at third order in QCD using the threshold approximation and the results for the associated production of Higgs boson with a vector boson computed at the same accuracy. We have demonstrated the numerical impacts in great detail for both the cases at LHC. We have found that the inclusion of such corrections do reduce theoretical uncertainties resulting from the renormalization scale.

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Journal

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3. Higgs Rapidity Distribution in $b\,\acute{b}$Annihilation at Threshold in N^3LO QCD, Taushif Ahmed, M. K. Mandal, Narayan Rana, V. Ravindran, *Journal of High Energy Physics*, 2015, 1502, 131
4. Associated production of Higgs boson with vector boson at threshold N^3LO in QCD, M. C. Kumar, M. K. Mandal, V. Ravindran, *Journal of High Energy Physics*, 2015, 1503, 037

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26. Name : **A. Masilamani Chelladurai**
Enrolment No. : ENGG02200904024
Date of Award of degree : 06.05.16
Constituent Institute : Indira Gandhi Centre for Atomic Research
Title : Study Of Pulsed Laser Seam Welding And Pulsed Laser-Gta Hybrid Welding On Aisi 316 Stainless Steel.

Abstract

Laser beam welding is an advanced welding process which found many advantages low heat input, deeper welds, high speed, ease of automation etc. The laser energy can be applied either in continuous or pulsed method. Pulsed mode lasers are utilized in precision weld applications as heat is applied as pulses of laser energy in controlled manner. In addition to spot welds, pulsed lasers are also used to make continuous welds by overlapping of spots, which is known as pulsed laser seam welding. There are two modes of energy transfer in laser welding namely conduction and keyhole. As different physical phenomena are involved in both the modes of operation, the resultant welds have distinct geometry and properties. Hence the process parameters which determine these modes need to be elucidated. In literatures, the transition from conduction to keyhole mode is considered to occur roughly at 10^6 W/cm^2. As many parameters involved in pulsed laser seam welding, this classification is not clearly understood to decide appropriate mode of operation. Pulsed laser welding of austenitic stainless steel which is a candidate material for nuclear applications is found to have solidification cracks. Further, this process address the challenges like the necessity of tight-fit up gap, low energy absorptivity, weld defects etc. The present work discusses energy transfer modes and its influence on solidification cracking in pulsed laser seam welding of stainless steels. It also comprises the studies on the development of pulsed laser-GTA hybrid welding, hybrid process parameters and comparative study of hybrid, laser and GTAW processes. The study clearly reveals that the conventional classification of modes derived from power density of 10^6 W/cm^2 is not applicable to pulsed laser seam welding. In a systematic study, different zones of energy transfer have been observed based on weld geometry and microstructures. The optimum pulse parameters have been identified to choose appropriate mode and to achieve deeper welds with efficient laser-material interaction. In addition to that for the first time, the effect of modes on

solidification cracking has been elucidated. Hybrid welding facility was developed and the effect of basic hybrid parameters on weld geometry has been studied to broaden the application window of pulsed laser seam welding. Drastic enhancement in depth of penetration, tolerance in fit-up gap, crack free welds have been observed. The mechanisms of augmentation in keyhole formation, pulsed laser-arc interaction and arc constriction under the influence of laser have been highlighted and discussed.

Publications

Journal

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2. Effect of Energy Transfer Modes on Solidification Cracking in Pulsed Laser Welding, A. M. Chelladurai, K. A. Gopal, S. Murugan, S.

3. Venugopal, S.K. Albert and T. Jayakumar, *Science and Technology of Welding and Joining*, **2015**, *20* (7), 578-584.

Conferences

1. A comparative study of GTAW and Laser Welding of Austenitic Stainless Steel Tubes, A. M. Chelladurai, K.A. Gopal, S. Murugan and S.K. Albert, *National Welding Seminar*- **2011**, Bhilai.

2. Development of Pulsed Laser- GTAW Hybrid Welding, A. M. Chelladurai, K.A. Gopal, S. Murugan, S. Venugopal and T. Jayakumar, *International Institute of Welding – International Welding Congress 2014 Proceedings*, **2014**, New Delhi, 171-176.

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27. Name : **Swagata Mallik**
Enrolment No. : PHYS04201204002
Date of Award of degree : 06.05.16
Constituent Institute : Variable Energy Cyclotron Centre
Title : Statistical And Dynamical Model Studies Of Nuclear Multifragmentation Reactions At Intermediate Energies

Abstract

Nuclear multifragmentation is an important phenomenon, the study of which can throw light on reaction mechanism in heavy ion collisions at intermediate and high energies. Based on statistical and dynamical model studies, this thesis is concentrated mainly on, the following three aspects of nuclear multifragmentation reactions namely (i) production of exotic nuclei which are normally not available in the laboratory (ii) nuclear symmetry energy from heavy ion collisions at intermediate energies and (iii) Nuclear liquid-gas phase transition. In addition to these equivalence of statistical ensembles under different conditions is also studied in the framework of multifragmentation.Projectile fragmentation is very useful for producing radioactive ion beams. A model for projectile fragmentation is developed and it is successfully applied to calculate different important observables and are compared with experimental data. A very simple impact parameter dependence of freeze-out temperature profile is introduced for understanding the reaction mechanism in the limiting fragmentation region. A microscopic static model and dynamical model based on Boltzmann-Uehling-Uhlenbeck equation is developed for determining the initial conditions (mass and excitation) of projectile fragmentation reactions. A hybrid model is also developed separately for explaining multifragmentation reaction reaction around Fermi energy domain.The underlying physical assumption behind canonical and grand canonical models is fundamentally different, and in principle it agrees only in the thermodynamical limit when the number of particles become infinite. Nevertheless, it is shown that these models are equivalent in the sense that they predict similar results if certain conditions are met even for finite nuclei. An analytical formula is derived which enables one to extract canonical results from a grand canonical calculation and vice versa.Study of nuclear symmetry energy in intermediate energy heavy ion reactions is an important area of research for determining the nuclear equation of state. In this thesis, symmetry energy coefficient is determined using different methods (isoscaling source method, isoscaling fragment method, fluctuation method and isobaric yield ratio method) in the framework of canonical and grand canonical models. It is observed that the best possible way to deduce the value of the symmetry energy is to use the fragment yield at the breakup stage of the reaction (not the “cold” fragments) as the secondary decay from higher energy states disturbs the equilibrium scenario.Another important area in the study of intermediate energy heavy ion collisions is the phenomenon of liquid gas phase transition. The standard methods of theoretical studies are based on statistical model calculations. This thesis focuses on whether results of transport model calculations (BUU) at intermediate energy can point to signatures of phase transition. To do that, a simplified yet accurate method of transport model is developed which allows calculation of fluctuations in systems much larger than what was considered feasible in a well-known and already existing model. The distribution of clusters is remarkably similar to that obtained in equilibrium statistical model and provides evidence of phase transition.

Publications

Journal

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2. “Improvements to a model of projectile fragmentation” S. Mallik, G. Chaudhuri and S. Das Gupta Physical Review C 84, 044612 (2011)

3. “Conditions for equivalence of statistical ensembles in nuclear multifragmentation” S. Mallik and G. Chaudhuri Physics Letters B 718 (2012) 189

4. “Symmetry energy from nuclear multifragmentation” S. Mallik and G. Chaudhuri Physical Review C 87 011602 (2013) (Rapid Communication)

5. “Transformation between statistical ensembles in the modeling of nuclear fragmentation” G. Chaudhuri, F. Gulminelli and S. Mallik Physics Letters B 724 (2013) 115

6. “Temperature of projectile like fragments in heavy ion collisions” S. Das Gupta, S. Mallik and G. Chaudhuri Physics Letters B 726 (2013) 427

7. “Effect of particle fluctuation on isoscaling and isobaric yield ratio of nuclear multifragmentation” S. Mallik and G. Chaudhuri Physics Letters B 727 (2013) 282

8. “Estimates for temperature in projectile-like fragments in geometrical and transport models ” S. Mallik, S. Das Gupta and G. Chaudhuri Physical Review C 89, 044614 (2014)

9. “Event simulations in a transport model for intermediate energy heavy ion collisions: Applications to multiplicity distributions” S. Mallik, S. Das Gupta and G. Chaudhuri Physical Review C 91, 034616 (2015)

10. “Hybrid model for studying nuclear multifragmentation around the Fermi energy domain: The case of central collisions of Xe on Sn” S. Mallik, G. Chaudhuri and S. Das Gupta Physical Review C 91, 044614 (2015)

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   S. Mallik, G. Chaudhuri and S. Das Gupta Proceeding of the DAE-BRNS Symposium on Nuclear Physics, Volume 56 (2011) 862.

2. “Study of the charge, mass and isotopic distribution in projectile fragmentation reactions” G. Chaudhuri, S. Mallik and S. Das Gupta
   Proceeding of the DAE-BRNS Symposium on Nuclear Physics, Volume 56 (2011) 760.

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28. Name : **Srikumar Sengupta**
Enrolment No. : PHYS07200604017
Date of Award of degree : 06.05.16
Constituent Institute : Institute of Physics,
Title : Aspects of QCD Phase Transition with Reaction-Difiusion Equations.

Abstract

This thesis is devoted to the study of the two important phase transitions associated with QCD, namely – chiral symmetry breaking transition and confinement-deconfinement transition. To that end, we have employed the techniques of reaction-diffusion equations to show that well-defined travelling front solutions, mimicking phase boundaries for a first-order transition, exist although the relevant QCD transitions are of second-order or a cross-over. We find that so long as dissipation dominates, a transition proceeds by a slow-moving front and a long-lasting mixed phase state prevails in the several fm time it takes to complete the transition. This is expected to leave its stamp on the various signals of QGP for RHICE, e.g. J/psi suppression, thermal photon and di-lepton production, quark-scattering (leading, perhaps, to baryon rich clusters), and, in particular, elliptic flow which develops mostly during the early stages. We have, further, considered the possibility of formation of disoriented chiral condensates (DCC), which were vigorously searched for in earlier experiments, in high multiplicity pp collisions at LHC energy. We argue that such high multiplicity collisions naturally give rise to the boundary conditions necessary for the existence of slowly propagating front solutions of reaction-diffusion equations with the resulting dynamics of the chiral field making sure that a large DCC domain is produced which gets stretched as the system expands and cools rapidly without a

significant roll-down of the chiral field. The subsequent decay of the DCC domain can lead to relatively clean signals of coherent pion emission.

Publications

Journal

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2 . Possibility of formation of a disoriented chiral condensate in pp collisions at energies available at CERN Large Hadron Collider via the reaction-diffusion equation. Partha Bagchi, Arpan Das, Srikumar Sengupta, Ajit M. Srivastava .Phys.Rev. C93 (2016) no.2, 024914; arXiv:1508.07752

3. Brane Solutions in Time Dependent Backgrounds in D = 11 Supergravity and in Type II String Theories. Srikumar Sen Gupt Int.J.Mod.Phys. A23 (2008) 2525-2540

4. Some new light-cone time dependent solutions in deformed pp-wave backgrounds. Srikumar Sen Gupta JHEP 05, 038 (2014)

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29. Name : **Uttam Bhunia**
Enrolment No. : PHYS04200904008
Date of Award of degree : 06.05.16
Constituent Institute : Variable Energy Cyclotron Centre
Title : Design and Optimization of Superconducting Magnet Systems for Energy Storage Application

Publications

Journal

1 U. Bhunia, S. Saha, A Chakrabarti, “Design optimisation of superconducting magnetic energy storage coil”, *Physica C,* 500 (2014) 25-32.

2 U. Bhunia, S. Saha, A Chakrabarti, “Pareto-optimal design of sector toroidal superconducting magnet for SMES”, *Physica C,* 505 (2014) 6-13.

3 U. Bhunia, J. Akhter, C. Nandi, G. Pal, S. Saha, “Design of a 4.5 MJ/1MW sectoredtoroidal superconducting Energy storage magnet”, *Cryogenics,* 63 (2014)186-198.

4 U. Bhunia, J. Pradhan, A. Roy, V. Khare, U. S. Panda, A. De, S. Bandopadhaya, T.Bhattacharyya, S. K. Thakur, M. Das, S. Saha, C. Mallik, R. K. Bhandari, “Design,Fabrication and Cryogenic Testing of 0.6 MJ SMES Coil”, *Cryogenics,* 52 (2012)719-724

30. Name : **Vishal Srivastava**
Enrolment No. : PHYS04201004005
Date of Award of degree : 06.05.16
Constituent Institute : Variable Energy Cyclotron Centre
Title : Study of Deuteron Induced Transfer Reactions on 27Al

Abstract

Single nucleon transfer reactions are good tools to extract spectroscopic information of nuclei. We can determine the excitation energy, spin and parity, orbital and total angular momentum. Study of transfer reactions also gives us opportunity to extract spectroscopic factors for single particle orbitals of the nuclei of interest. Being fundamental property of a nucleus, spectroscopic factors should be independent of incident energies as well as involved reactions. In the present thesis work, we have studied different states of ^{26}Al and ^{26}Mg observed through the reactions ^{27}Al(d,t) and ^{27}Al(d,^{3}H), respectively. To study different states of ^{26}Al and ^{26}Mg, the experiment was performed at the Variable Energy Cyclotron Centre, Kolkata using deuteron beam of energy 25 MeV on a self - supporting target ^{27}Al (~90 μg/cm^{2}). In this experiment, a three element detector telescope system, consisting of a single - sided 55 μm thick Si (ΔE) strip detector, a double - sided 1030 μm Si (E) strip detector and four CsI(Tl) detectors (each of thickness 6 cm) has been used for identification of different particles. The angular distributions of the ejectiles were measured in the angular range of 16 to 40 in steps of 0.9 . Several excited states of ^{26}Al and ^{26}Mg were populated through the reactions ^{27}Al(d, t) and ^{27}Al(d, ^{3}He), respectively. A VME based data acquisition system (DAQ) developed at VECC was used to collect the online event by event data. The offline data extraction and analysis was performed using different algorithm developed in ROOT platform. The ECIS94 optical model search code has been used to extract optical model potential parameters from the angular distribution of the elastically scattered deuterons. Zero range distorted wave Born approximation calculation has been performed using the computer code DWUCK4 for the analysis of the observed states of ^{26}Al and ^{26}Mg. The experimentally extracted angular distributions of the cross sections of different observed states of ^{26}Al and ^{26}Mg were compared with respective theoretically predicted cross sections from DWUCK4 code to extract spectroscopic factors. The present study of the different states of ^{26}Al through 1n pickup reaction ^{27}(d,t) is the first direct study of ^{26}Al using (d,t) reaction channel. The extracted spectroscopic factors of the observed states of ^{26}Al in the present study were compared with previously reported values for the same using different reaction probes as well as with those predicted theoretically for the same and were found to be in good agreement. As the spectroscopic factors of isobaric analog states (IAS) in isobaric multiplets should be identical, so the low lying T = 1 IAS of ^{26}Al and ^{26}Mg were also investigated for the first time using ^{27}Al(d, t / ^{3}He) reaction sequence and the result confirms their analog. characteristics Apart from investigation of low lying T = 1 IAS, the extracted spectroscopic factors of the observed states of ^{26}Mg were also compared with previously reported values using the same reaction probe for the same at different energies and were found to be in consistent with each other. The results of the present study were also compared with theoretical predictions available in literature for the same nuclei and were also found to be in agreement.

Publications

Journal

1. *"Experimental study of ^{26}Al through the 1n pick up reaction ^{27}Al(d,t)"*: Vishal Srivastava, C. Bhattacharya, T. K. Rana, S. Manna, S. KunduS.Bhattacharya, K. Banerjee, P. Roy, R. Pandey, G. Mukherjee, T. K. Ghosh, J. K. Meena, T. Roy, A.Chaudhuri, M. Sinha, A. Saha A. Dey, Md. A. Asgar, Subinit. Roy, and Md. M. Shaikh. Phys. Rev. C 91, 054611 (2015).

2. *"Experimental investigation of T = 1 analog states of ^{26}Al and ^{26}Mg"*:VishalSrivastava, C. Bhattacharya, T. K. Rana, S. Manna, S. Kundu, S Bhattacharya, K. Banerjee, P. Roy, R. Pandey, G. Mukherjee, T. K. Ghosh, J. K. Meena, T. Roy, A.Chaudhuri, M. Sinha, A. Saha A. Dey, Md. A. Asgar, Subinit. Roy, and Md. M. Shaikh. Phys. Rev. C 93, 044601 (2016).

3. *"Study of ^{26}Mg through the 1p pick up reaction ^{27}Al(d,^{3}He)"*: Vishal Srivastava, C. Bhattacharya, T. K. Rana, S. Manna, S. Kundu, S Bhattacharya, K. Banerjee, P. Roy, R. Pandey, G. Mukherjee, T.K. Ghosh, J. K. Meena, T. Roy, A.Chaudhuri,M. Sinha, A. Saha A. Dey,Md. A. Asgar, Subinit. Roy, and Md. M. Shaikh. arXiv:1510.04416.

4. *"Structure of ^{26}Al studied by one -nucleon transfer reaction ^{27}Al(d,t)"*: Vishal Srivastava, C. Bhattacharya, T. K. Rana, S. Manna, S. Kundu, S.Bhattacharya, K. Banerjee, P. Roy, R. Pandey, G. Mukherjee, T.K. Ghosh, J. K. Meena, T. Roy, A.Chaudhuri,M. Sinha, A. Saha A. Dey,Md. A. Asgar, Subinit. Roy, and Md. M. Shaikh. EPJ Web of Conferences 86, 00055 (2015).

5 *"Excited states of ^{26}Al studied via the reaction ^{27}Al(d,t)"*: Vishal Srivastava, C. Bhattacharya, T. K. Rana, S. Manna, S. Kundu, S. Bhattacharya, K. Banerjee, P. Roy, R. Pandey, G. Mukherjee, T.K. Ghosh, J. K. Meena, T. Roy, A. Chaudhuri,M. Sinha, A. Saha A. Dey,Md. A. Asgar, Subinit. Roy, and Md. M. Shaikh. To be published in EPJ Web of Conferences (Accepted; in press).

Conference Proceedings:

1. *"Study of one neutron pick-up reaction ^{27}Al(d,t)"*:Vishal Srivastava, C. Bhattacharya, T. K. Rana, S. Manna, S. Kundu, S. Bhattacharya, K. Banerjee, P. Roy, R. Pandey, G. Mukherjee, T.K. Ghosh, J. K. Meena, T. Roy, A.Chaudhuri,M. Sinha, A. Saha A. Dey,Md. A. Asgar, Subinit. Roy, and Md. M. Shaikh. Proceedings of the DAE Symp.onNucl. Phys. 59, 358 (2014).

2. *"Study of one proton pick-up reaction ^{27}Al(d,^{3}He)"*: Vishal Srivastava, C. Bhattacharya, T. K. Rana, S. Manna, S. Kundu, S. Bhattacharya, K. Banerjee, P. Roy, R. Pandey, G. Mukherjee, T. K. Ghosh, J. K. Meena, T. Roy, A.Chaudhuri, M. Sinha, A. Saha A. Dey,Md. A. Asgar, Subinit. Roy, and Md. M. Shaikh. Proceedings of the DAE Symp.onNucl. Phys.60, 342 (2015).

31. Name : **Eshita Mazumdar**
Enrolment No. : MATH08201004001
Date of Award of degree : 09.05.16
Constituent Institute : Harish-Chandra Research Institute
Title : Algebraic And Combinatorial Methods In Zero-Sum Problems.

Abstract

For a finite abelian group Gwith exp(G) = n and A to be a non-empty subset of {1,2,...,n-1}, the arithmetical invariant $s_{mn,A}(G)$ is defined to be the least integer k such that any sequence S with length k of elements in G has a A-weighted zero-sum subsequence of length mn. When m =1 and A = {1} it is the *Erdős-Ginzburg- Ziv* constant and is denoted by s(G). Another invariant $_A(G)$ is defined to be the smallest positive integer t such that any sequence of elements t contains a non-empty A-weigthed zero-sum subsequence of length at most exp(G). This generalizes the constant (G) which corresponds to the case A={1}. In the first part of my dissertation for the cyclic group Z_n, I have modified a method of Griffiths which had been used to attack a problem for some weighted version of the constant. After doing this I was mainly interested about that how this invariant behaves for higher dimensional cases. I have found very interesting results for higher dimensional cases by keeping the weight set A={1, -1}. The rest of my thesis is focused on finding out the relationship between the weighted zero-sum invariants $s_A(G)$ and $_A(G)$.

Publications

Journal

1. "Modification of some methods in the study of zero-sum problems",Sukumar Das Adhikari, EshitaMazumdar, Integers (2014) 14, #A25.
2. "The polynomial method in the study of zero-sum theorems", Sukumar Das Adhikari, EshitaMazumdar, Int. J. Number Theory (2015), Vol. 11, No. 5, 1451-1461.
3. "Relations between two zero-sum constants", Sukumar Das Adhikari, EshitaMazumdar, B. K. Moriya. (accepted in "Integers").

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32. Name : **Jedidiah Pradhan**
Enrolment No. : PHYS04200904007
Date of Award of degree : 20.05.16
Constituent Institute : Variable Energy Cyclotron Centre
Title : Thermo-dynamical study of steady state and transient process in a dilution refrigerator

Abstract

A thermal model of dilution refrigerator is formulated using numerical simulation program SIDFO (Simulation of Integrated Dilution refrigerator For Optimization. It can simulate varying process parameters and can be used for calculations prior to any process modifications. In addition it allowed us to carry out a

comprehensive study of time dependent analysis of transitory phase. Furthermore, with this approach new process equipments can be easily added. While many analyses and models of the thermo-dynamical process related to dilution refrigerator already exist, the present work describes the congregation of all components of the dilution refrigerator making up a complete closed cycle simulation. The simulation is further upgraded to accommodate the stages of development preceding the steady state condition by introducing time dependent variations. To our knowledge, no comprehensive study to investigate the time dependent manifestation of transitory phases in dilution refrigerator has been done earlier. Moreover, simulation has produced several unique results of the underlying phenomena occurring at various stages of the low temperature process. Thermo dynamical analysis of steady state and transient processes through SIDFO has helped to conceptualize and design a complete dilution refrigeration system. The dilution refrigerator was successfully built and temperature down to below 50mK have been achieved and maintained for hours. The results of simulation as well as results based on other existing models are compared with experimental data derived from measurements.

Publications

Journal

1. Jedidiah Pradhan, Nisith K. Das and Alok Chakrabarti, "Transient phenomena initiating phase transition in dilution refrigerator", Cryogenics (2014) 63, 69-76.
2. Jedidiah Pradhan, Nisith K. Das and Alok Chakrabarti, "Thermodynamic process simulation of dilution refrigerator", Cryogenics (2013) 57, 158-165.
3. N.K. Das, J. Pradhan, et al, "Design and performance of a ^{4}He-evaporator at < 1.0K ", Cryogenics (2012) 52,679-684.
4. N.K Das, J. Pradhan, et al, "Design Optimization of 1K-Helium Evaporator", Indian. Jour. of Cryogenics, 36(2011), 55-57.

Conferences/symposiums:

1. N.K Das, J Pradhan et al., " Three stage vacuum system for ultralow temperature installation" published in IOP Journal of Physics: Conference series 390 (2012) 012055.
2. N.K Das, J Pradhan et al., "Indigenous development of technologies relevant to milli-kelvin facility at VECC, Kolkata", presented in 25th National Symposium on Cryogenics (NSC-25), December 8-10, 2014, Hyderabad, India.
3. J. Pradhan et. al., " Thermodynamic Process Simulation of Dilution Fridge", presented in Asian Conference on Applied Superconductivity and Cryogenics 2011 (ACASC-2011), New Delhi, India.
4. N.K Das, J Pradhan et al., "Indigenous development of a dilution refrigerator", presented in 26th International Cryogenic Engineering Conference (ICEC-2016) in New Delhi, India.

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1. Jedidiah Pradhan, Malay Kanti Dey and Alok Chakrabarti, "A Generalized Formulation of Beam-Shadow Measurement in Spiral-Sector Superconducting Cyclotron", published in Nuclear Instruments and Methods in Physics research section A (NIM-A), volume 748, 2014(p79-83).

2. J.Pradhan et. al., "Basic design and test results of HTS insert Coil for high field hybrid magnet", Current Science Vol. 104, No 9, p1142-1146, 2013.
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4. T Bhattacharjee, MK Dey, P Dhara, S Roy, J Debnath, RB Bhole, A Dutta, J Pradhan et al., “Development of Fast Scintillator based Beam Phase Measurement System for Compact Superconducting Cyclotron”, Review of Scientific Instruments 84 (2013).
5. J Pradhan et. al., "Design and Development of HTS Magnet Insert to produce 12T of Magnetic field" published in Indian Journal of Cryogenics Vol. 37 No 1-4, 2012.
6. J Pradhan et. al., “Design, Fabrication and Testing of HTS based Current Lead ", published in Indian Journal of Cryogenics Vol. 36 No 1-4, 2011.

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33. Name : **Sumana Paul**
Enrolment No. : CHEM01201004015
Date of Award of degree : 20.05.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Development Of Polymeric Sorbent Based Analytical Methods For Actinides.

Abstract

The work described in this thesis involves development of bi-functional polymeric sorbents for selective preconcentration of major actinides (U, Pu), followed by the direct quantification of the actinide sorbed the polymeric substrate by either alpha spectrometry or mass spectrometry. Two bi-functional polymers, HEMP-co-AMPS and HEMP-co-APTAC, were synthesized by photo-induced free radical polymerization using monomers phosphoric acid 2-hydroxyethyl methacrylate ester (HEMP) with either 3-(acrylamidopropyl)trimethylammonium chloride (APTAC) or 2-acrylamido-2-methyl-1-propanesulphonic acid (AMPS). These bi-functional polymers, containing neutral phosphate groups and strong ion-exchange groups i.e. either sulphate or quaternary ammonium groups, were found to be selective for a particular actinide depending on the HNO_3 concentration of the medium. Both HEMP-co-AMPS and HEMP-co-APTAC had better extraction and stripping properties compared to HEMP polymer and were found to sorb Pu(IV) preferentially in the presence of large excess of U(VI) ions. The HEMP-co-AMPS polymer was anchored as a thin film on the surface of poly(ethersulphone) membrane, which served as a good source for quantification of Pu(IV) in complex aqueous matrices by alpha spectrometry. Membrane based alpha spectrometry was employed for determination of trace amounts of Pu(IV) in various biological & environmental samples and in dissolver solution, containing large excess of U. Single bead thermal ionization mass spectrometry (SB–TIMS) was developed for simultaneous preconcentration of plutonium using magnetic bifunctional PES beads, followed by determination of Pu isotopic composition and concentration. The method significantly reduces the analysis time & the amount of solid/liquid waste generated is minimized. However analysis temperature of SB–TIMS was found to be considerably higher than the conventional solution based TIMS method. To overcome such problem, the liquid extractants HDEHP and TEHP were physically immobilized in the poly(propylene) membrane to serve dual functions i.e. efficient preconcentration of Pu(IV) and U(VI) from a wide variety of aqueous matrices and TIMS loading with low vaporization temperature. Membrane based TIMS was applied successfully for the quantification U(VI) and Pu(IV) in the synthetic urine sample, seawater and ground water using isotope dilution method with reasonable good accuracy and precision. The major advantage of the Reservoir-TIMS developed in the present work is that it is a single step sample manipulation and loading process that would greatly reduce the analysis time and prolong handling of the radioactivity causing possibility of contamination and exposure to radiations.

Publications

Journal

1. Tailored bi-functional polymer for actinides monitoring;Sumana Paul, Ashok K. Pandey, Pranaw Kumar, Santu KaitS.KAggarwal; Analytical Chemistry, 86 (13), 2014, 6254–6261.

2. Chemically selective polymer substrate based direct isotope dilution alpha spectrometry of Pu; Sumana Paul, Ashok K. Pandey, R.V. Shah and S.K. Aggarwal;Analytica Chimica Acta, 878 (2015) 54–62.

3. Superparamagnetic bi-functional composite bead for thermal ionization mass spectrometry of plutonium(IV) ions;Sumana Paul, Ashok K. Pandey, Raju V. Shah, D. Alamelu and Suresh K. Aggarwal; RSC Advances, 6 (2016) 3326–3334.

4. Polymeric material based reservoirs for thermal ionization mass spectrometric determination of uranium(VI) and plutonium(IV) ions in environmental and process aqueous samples;Sumana Paul, Ashok K. Pandey, Raju V. Shah, K. Sasi Bhusan and Suresh K. Aggarwal;Journal of Analytical Atomic Spectrometry, 31 (2016) 985–993.

Symposium

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2. Development of phosphate functionalised sorbents for selective preconcentration of Actinides;Sumana Paul, Pranaw Kumar, A.K. Pandey and S.K. Aggarwal; Proc. of 11th DAE-BRNS NUCAR 2013 Symposium, B-17, p. 211.

3. Membrane based Isotope Dilution Alpha Spectrometry (MEM–IDAS) for Determination of Plutonium concentration;Sumana Paul, R.V. Shah, A.K. Pandey and S.K. Aggarwal; Proc. of NAC-V 2014 symposium, Paper No. D-40, Page 304.

4. Gel based loading for determination of Pu isotopic composition by Thermal Ionization Mass Spectrometry;Sumana Paul, R.V. Shah, A.K. Pandey and S.K. Aggarwal; Proc. of 28th ISMAS-WS-2014, Paper CP-32, Page 238.

5. Membrane based isotope dilution alpha spectrometry for determination of plutonium concentration;Sumana Paul, R.V. Shah, A.K. Pandey and S.K. Aggarwal; Proc. of ISMC-2014, Paper No. A–127, p. 110.

6. Selective extraction of plutonium from nitric acid medium by bifunctional polyethersulfone beads for quantification with thermal ionisation mass spectrometry;Sumana Paul, A.K. Pandey and S.K. Aggarwal; Proc. of NUCAR-2015, Paper No. E-46, Page No. 393.

7. Resin bead-thermal ionization mass spectrometry for determination of plutonium concentration in irradiated fuel dissolver solution;Sumana Paul, R.V. Shah, A.K. Pandey and S.K. Aggarwal; Proc. of 29th ISMAS-WS-2015, Paper No. CP-30, Page No. 173.

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34. Name : **Jitesh Singh Rathee**
Enrolment No. : LIFE01200804010
Date of Award of degree : 20.05.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Effect Of A Natural Compound Malabaricone C, On Cardiovascular Disease And Remodeling.

Abstract

Cardiovascular disease (CVD) mediated pathogenesis affects heart, kidney and blood vessels. India has the dubious distinction of being known as the coronary and diabetes capital of the world. By 2020, CVD is likely to become the single leading cause of death and disability in India. Major contributing factors to CVD are hypertension (HT), hypertrophy, endothelial dysfunction and electrical remodeling. The clinically used drugs against HT and CVD have several side effects, and does not produce desired end results, warranting search for newer alternatives possibly from natural and dietary sources. To this end, I have analyzed the cardiovascular remodeling property of malabaricone C (mal C), a natural phenolic constituent of *Myristica malabarica* in the DOCA-salt hypertensive (DSH) rat model which shows severe pathological cardiovascular remodeling. In rat, mal C administered orally, was found to be nontoxic and fairly bioavailable. It reduces the hypertension and increases the survival rate of DSH rats in a concentration dependent manner. Therapeutic administration of mal C to DSH rats significantly attenuated the rise in hypertrophy, fibrosis, atrial natriuretic peptide and inflammation in cardiac and aortic tissues. It also reduces plasma Na$^+$ and Ca^{2+} levels, vasoconstrictors (big endothelin, endothelin-1 and arg^8-vasopressin), tissue oxidative damage and passive diastolic stiffness in perfused hearts. It improves the vascular reactivity against vasoconstrictors and vasorelaxants. Besides, mal C also restricted the prolongation of action potential durations of repolarization in papillary muscle, decrease in the plasma K$^+$ concentrations, reduction in eNOS expression and vascular dysfunction in DSH rats. It also corrects the changes in QRS, QTc, P, PR durations, and heart rate of DSH rats as revealed by ECG profiles. The cardiac structural and functional parameters with improved diastolic filling along with the cardiac output of DSH rats were also improved by the mal C administration as evident by the ECHO analysis. Overall, it increased the antioxidant status and survivability of the DSH rats. The results suggested that mal C can be a potential fairly absorbed, non-toxic cardiovascular protecting agent.

Publications

Journal

1. Mechanism of the anti-hypertensive property of the naturally occurring phenolic, malabaricone C in DOCA-rats. Jitesh S. Rathee, Birija S. Patro, Lindsay Brown, and Subrata Chattopadhyay. *FRR Volume 50, Issue 1, 2016, DOI: 10.3109/10715762.2015 .1112005.*

2 Cardiovascular remodulatory effect of a naturally occurring phenolic, malabaricone C in DOCA-rats. Jitesh S. Rathee, Lindsay Brown, and Subrata Chattopadhyay. Manuscript communicated to *Pharmacology Research.*

Conferences

1. Targeting cardiovascular disease with a novel dietary molecule, malabaricone C. INVITED Lecture. Jitesh Rathee and S. Chattopadhyay. *International Conference on Cardiovascular*

Translational Research and the 13th Annual Conference of ISHR (Indian Section). Jan 22-24, 2016, IIT Madras, Chennai, India.

2. Cardiovascular remodeling property of a malabaricone C in DOCA-salt hypertensive rats. Jitesh Rathee and S. Chattopadhyay. in *International Symposium on Advances In Free Radicals, Redox Signaling And Translational Antioxidant Research (SFRR-STAR).* Lucknow (Jan 2013)
3. Antihypertensive activity of a natural phenolic malabaricone C in DOCA-salt rats. Jitesh Rathee and S. Chattopadhyay. in *International Conference on Recent Advances In Free Radical Research, Natural Products, Antioxidants & Radio-protectors In Health*. Hydrabad (Jan 2010)

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35. Name : **Neha Trivedi**
Enrolment No. : ENGG01201204016
Date of Award of degree : 27.05.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Evolution of Size Independent Fracture Energy through Characterization of Fracture Process Zone in Concrete Structures.

Abstract

Fracture in concrete, results from the coalescence of micro-cracks and formation of a Fracture Process Zone (FPZ) and further development of macro-cracks leading to fracture propagation. The size of the FPZ in front of an existing crack or notch determines the extent of energy dissipated during fracture. Studies on the concrete fracture energy, FPZ, the behavior of concrete during fracture process and size effect are at the forefront of research on concrete fracture. The main objective of this study is to present various approaches for the investigation of the size independent fracture energy (*GF*) of concrete and characteristics of FPZ to address the important features of crack formation and its propagation in quasi-brittle material like concrete. This study leads to establish a size independent fracture energy that can be used as a material parameter in the numerical analysis of concrete structures. The fracture energy and FPZ are the most useful parameters for characterizing the fracture behavior and analysis of concrete structures. The numerical modelling of Three Point Bend (TPB) concrete beams that are geometrically similar having constant length to depth ratio with varying range of notch to depth (*a/D*) ratios is performed. The unique non-linear behavior of concrete material is incorporated through fracture energy based softening model in the finite element numerical simulation. In the numerical study of concrete components, mesh sensitivity is an extremely important issue, which has been addressed in this work. In the present finite element analysis of TPB fracture test, the performance of triangular elements is investigated and observed to be superior over the quadrilateral elements for fracture analysis. The RILEM fracture energy (*Gf*) values evaluated by load-load line displacement responses obtained experimentally and through the numerical simulation of several set of experiments are beset with size effects. *Gf* values are utilized to determine *GF* by Hu and Wittmann method based on bilinear model. In addition, the fact as reported in literature that ratio of fracture energy to the uncracked ligament length almost becomes constant at larger uncracked ligament lengths is proved in this study. Further, relationship based on fracture energy release rate is developed to assess the *GF*. Another methodology based on averaging of *Gf* values associated with geometrically similar beams, is developed for the evaluation of size independent fracture energy of concrete. The fracture parameters through Bazant's

size effect studies and Jenq-Shah size effect law are investigated. FPZ is visualized for notched concrete beams under bending using a testing scheme called Digital Image Correlation (DIC). A new approach known as Optical Crack Profile (OCP), based on DIC experiments, is proposed to quantify the fracture parameters such as crack opening displacement, width of FPZ, length of FPZ and fracture energy. A comprehensive analysis of fracture energy estimated from various methodologies such as bilinear model, fracture energy release rate, *Gf* averaging for geometrically similar beams, Bazant size effect laws, Jenq-Shah model and OCP technique have been carried out to obtain a unique value of the size independent fracture energy of concrete.

Publications

Journal

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2. Characterization of concrete specimen fracture response: 2D numerical study. N. Trivedi, R. K. Singh and J. Chattopadhyay. *Structures*. 2015. 1. 39-50.
3. A comparative study on three approaches to investigate the size independent fracture energy of concrete. N. Trivedi, R. K. Singh and J. Chattopadhyay. *Engineering Fracture Mechanics*. 2015. 138. 49-62.
4. Investigation on fracture parameters of concrete through Optical Crack Profile (OCP) and size effect studies. N. Trivedi, R. K. Singh and J. Chattopadhyay. *Engineering Fracture Mechanics*. 2015. 147. 119-139.

International Conference: 02

1. Size Independent Concrete Fracture Energy Investigation. N. Trivedi, R. K. Singh and J. Chattopadhyay. 5th *International Congress on Computational Mechanics and Simulation* (ICCMS).10-13 December. 2014. SERC Chennai. India.

2. Numerical Modelling For Characterizing Concrete Fracture Parameters. N. Trivedi, R. K. Singh and J. Chattopadhyay. 5th *International Congress on Computational Mechanics and Simulation* (ICCMS). 10-13 December. 2014. SERC Chennai. India

36. Name : **Anoop Varghese**
Enrolment No. : PHYS10200604015
Date of Award of degree : 19.09.13
Constituent Institute : Bhabha Atomic Research Centre
Title : Evolution of Size Independent Fracture Energy through Characterization of Fracture Process Zone in Concrete Structures

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37. Name : **Thomas Paul V.**
Enrolment No. : ENGG02200804022
Date of Award of degree : 27.05.16
Constituent Institute : Indira Gandhi Centre for Atomic Research
Title : Evolution Of Microstructure And Correlation With Properties In Weldments Of 9cr Reduced Activation Ferritic / Martensitic Steels.

Abstract

This thesis titled "Evolution Of Microstructure And Correlation With Properties In Weldments Of 9cr Reduced Activation Ferritic / Martensitic Steels" presents the results of a systematic study on the physical metallurgy aspects of two variants of RAFM steel with different W contents with emphasis on the microstructures that evolve in this steel on heat treatment and welding employing a variety of characterization techniques. The evolution of microstructures was studied by both computation and experimental methods. The consequence of microstructural variation on the mechanical properties of the steel has been studied using impression creep and small punch techniques. Microstructural evolution in RAFM steels during thermal exposures was studied in detail with respect to alloy composition, evolution of phases and influence of secondary phases on mechanical properties. Higher tungsten content in INRAFM steel delayed the coarsening of carbides and growth of laths. Coarsening of MX was negligible in both the steels. Computation by JMatPro® calculated the existence of M_2X carbo-nitrides only up to 4 h of heat treatment at 873 K. A progressive enrichment of Cr is observed in $M_{23}C_6$ upon aging, also supported by computation. JMatPro® predicted the nucleation of Laves phase at 773 K in 1W RAFM steel. But no experimental evidence could be obtained even after 10000 h of aging which is attributed to kinetic factors. Laves phase nucleates at 823 K in INRAFM steel and forms as a continuous network around ~10000 h of aging. Creep properties of the two steels in normalized tempered condition were compared using impression creep test. Change in creep rate on aging of INRAFM is estimated and correlated with coarsening of carbides and formation of Laves phase.The study on different welding methods includes the variation in microstructural parameters in welds prepared by different methods. Decrease in hardness across the HAZ is understood based on the decreasing peak temperature, which dictates the extent of carbon super saturation and dislocation density in the martensite. Thermal cycling experienced by different regions of autogenous weldment was calculated using Rosenthal's steady state solutions to heat transfer equation. Weld metal of TIG joint showed a coarser PAGS compared to EB and LB welds due to the higher residence time at temperatures above A_{c3}. Temperature-time window for the formation of Laves phase in various regions of RAFM steel weldments have been identified by JMatPro based computations. Experimental results indicate the formation of Fe_2W type Laves phase in FGHAZ of INRAFM steel at an early stage of exposure to temperatures $\geq$823 K. This is attributed to the abundant carbide precipitations in this region leading to an increase in W and decrease in C content locally which does favor nucleation and growth of Laves phase.

Laves phase could not be detected in 1W-RAFM steel under identical experimental conditions.The study on RAFM-316L dissimilar welds joint, brought out different microstructural zones in the dissimilar weld and evolution of microstructure during PWHT & aging. The experimental results of EBSD were found to be in line with Schaeffler diagram which predicted a duplex microstructure of martensite and austenite in the weld metal. The presence of delta ferrite at the austenite interface was identified by XRD and EBSD techniques. The reversion of martensite after PWHT and long term heat treatment could be explained on the lowering of transformation temperatures due to diffusion of Cr and Ni into weld metal.

Publications

Journal

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2. Influence of alloy content and prior microstructure on evolution of secondary phases in weldments of 9Cr Reduced Activation Ferritic-Martensitic steel, V. Thomas Paul, C. Sudha, S. Saroja; Metall. Mater. Trans.A, 46 (8) (2015) 3378-3392.

3. Microstructural variations across a dissimilar 316L austenitic - 9Cr Reduced Activation Ferritic Martensitic steel weld joint: V. Thomas Paul, Karthikeyan T, Arup Dasgupta, Sudha C, Hajra R.N, Shaju K. Albert, S. Saroja and Jayakumar T, Metall. Mater. Trans.A, 47A (3) (2016), 4432-1168.

Conference presentation:

1. Early precipitation of laves phase in the heat affected zone of 9cr RAFM steel weldment; V. Thomas Paul, S. Saroja, T. Jayakumar, E. Rajendra Kumar, Proc. International Conf. Electron Microscopy, EMSI 2013, (2013) Kolkata p.203.

2. Effect of Tungsten on microstructural evolution and mechanical properties of 9Cr RAFM steel; V. Thomas Paul, Ran Vijay Kumar, V. D. Vijayanand, V. Karthik, C. Sudha and S. Saroja , 7th International Conference on Creep, Fatigue and Creep Fatigue Interaction (CF-7)

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38. Name : **Roji Pius**
Enrolment No. : PHYS08201004003
Date of Award of degree : 27.05.16
Constituent Institute : Harish-Chandra Research Institute
Title : Perturbative Aspects Of String Theory And Gauge/String Duality.

Abstract

Main goal of this thesis is an improved understanding of string theory and gauge/gravityduality by looking into the perturbative aspects of it. Below we list the major results of thestudies that will be presented in this thesis.

- We found a consistent prescription for computing the renormalized masses and S-matrixelements of string states whose masses are not protected by any symmetry.
- We determined the stability of massive non-BPS SO(32) spinor in SO(32) heterotic string theory compactified on circle in the entire moduli space which is parameterized by the radius of

compactification and string coupling.

- As a modest step towards understanding the inner working of gauge/string duality westudied a simple example of gauge/string duality. We found thematching of leading order terms in a class of correlators of this conjectured dualitybetween topological A-model string theory on CP1 and gaussian matrix models. We alsofound a nice interpretation for the mismatch in the sub-leading terms.

Publications

Journal

1. "Mass Renormalization in String Theory: Special States", Roji Pius, ArnabRudra,Ashoke Sen, Journal of High Energy Physics, 2014, Vol. 1407(2014)058.
2. " Mass Renormalization in String Theory: General States", Roji Pius, Arnab Rudra, Ashoke Sen, Journal of High Energy Physics, 2014, Vol. 1407(2014)062.
3. "S-duality Improved Perturbation Theory in Compactified Type I/Heterotic String Theory.", Roji Pius, Ashoke Sen, Journal of High Energy Physics, 2014, Vol.1406(2014)068.
4. " Mass Renormalization in String Theory: General States", Rajesh Gopakumar, Roji Pius, Journal of High Energy Physics, 2013, Vol. 1303(2013)175.

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39.	Name	:	**Rakhi Paul**
	Enrolment No.	:	LIFE05200904001
	Date of Award of degree	:	27.05.16
	Constituent Institute	:	Saha Institute of Nuclear Physics,
	Title	:	Structure-Function Relationship Of Sugar Kinases From Vibrio Cholerae O395.

Abstract

The work explained in the thesis contains detailed structural, biochemical and biophysical characterization of two sugar kinases, namely Ribokinase (VcRK) and Fructokinase (VcFK). The thesis contains five chapters. The first chapter elucidates a brief review of literature of sugar kinase families and the relevance of choosing the two kinases. The second chapter describes the materials and methods used in the studies. The third chapter explains the detailed result of cloning, over-expression, crystallization, data collection of VcRK and VcFK. the detailed enzyme kinetic data of VcFK including roles of monovalent and divalent cations are also discussed in the chapter. The fourth and fifth chapters present the structural details of VcRK and VcFK with the help of crystal structures of both kinases in apo form and corresponding sugar-ATP-analog bound form. The structural studies include dimerization, sugar binding, and large scale loop movements during sugar binding and monovalent/divalent cation binding. Although same loops are involved in dimerization of both enzymes, the dimerization of VcRK and VcFK are widely different. In VcRK, two dimerization loops from neighbouring monomers compose β-clasp motif whereas in VcFK dimerization region is rather flat. Structural comparison of apo and sodium ion bound structures in VcFK explains the structural basis of activation of fructokinase by monovalent cation. The octahedral geometry of calcium ion binding site has been analyzed carefully. High fidelity of phosphotransfer reaction is gained by involvement of dimerization loops from either same monomer (VcFK) or neighbouring monomer (VcRK). In VcFK, a high resolution structure (1.29Å) containing fructose, ADP and BeF_3 provide the picturesque detail of the transition state before phosphotransfer. The roles of conserved residues are discussed thoroughly for ribokinase superfamily.

Publications

Journal

i) Paul R, Patra MD, Sen U. Crystal Structure of Apo and Ligand Bound Vibrio cholerae Ribokinase (Vc-RK): Role of Monovalent Cation Induced Activation and Structural Flexibility in Sugar Phosphorylation. Adv Exp Med Biol.2015; 842:293-307.

ii) Paul R, Patra MD, Banerjee R, Sen U. Crystallization and preliminary X-ray analysis of a ribokinase from Vibrio cholerae O395. Acta Crystallogr F Struct Biol Commun. 2014 Aug; 70 (Pt 8):1098-102.

iii) Paul R, Nath S, Sen U. Cloning, expression, purification, crystallization and preliminary X-ray analysis of a fructokinase from Vibrio cholerae O395. Acta Crystallogr Sect F Struct Biol Cryst Commun. 2012 Dec 1;68(Pt 12):1564-7.

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40. Name : **M.L. Jayalal**
Enrolment No. : ENGG02200804016
Date of Award of degree : 27.05.16
Constituent Institute : Indira Gandhi Centre for Atomic Research
Title : Application Of Genetic Algorithm Based Optimization Methodologies To Some Of The Systems Of Indian Nuclear Reactors.

Abstract

The study carried out in the thesis was motivated by the need to develop and compare suitable Genetic Algorithm optimization methodologies for application of problems in diverse reactor environments. As part of the study, suitable Genetic Algorithm based methodologies are applied and evaluated in a set of diverse and less explored reactor environments of Pressurized Heavy Water Reactor and Fast Breeder Reactor. The subsystems of reactors selected are: (i) steam condenser of Prototype Fast Breeder Reactor (PFBR) (ii) burnup zones of the core of a 220 MWe Pressurized Heavy Water Reactor (PHWR) (iii) fuel enrichment zones of the cores of a 500 MWe Fast Breeder Reactor (FBR)(iv) fuel enrichment zones of the cores of a 1000 MWeFBR. The suitability of different methodologies of the Genetic Algorithm namely, Penalty-function GA and Multi-objective GA, for different types of nuclear fuel management optimizations are studied and compared in the work.The evaluation of these methodologies for reactor applications is a novel initiative highlighted in this work. The study also explores in identifying the appropriate choice of Genetic Algorithm methodology for a particular reactor application. The results obtained from the studies carried out as part of the thesis clearly establishes the suitability of the selected Genetic Algorithm methodologies, in the optimization studies related to different nuclear reactor systems. A modular approach has been followed and applied in developing the optimization methodologies based on the Genetic Algorithms.This approach has provided the possibility of developing more efficient communication mechanisms and the flexibility in modifying the modules for extending the applications to other reactor systems.

Publications

Journal

1. Steam Condenser Optimization using Real Parameter Genetic Algorithm for Prototype Fast Breeder ReactorM.L. Jayalal, L. Satish Kumar, R. Jehadeesan, S. Rajeswari, S.A.V. SatyaMurty, V. Balasubramaniyan, S.C. Chetal
Nuclear Engineering and Design 241(2011) 4136-4142

2. Computational Intelligent Systems for Prototype Fast Breeder ReactorM.L. Jayalal, T. Jayanthi, S.A.V. SatyaMurty, P. Swaminathan*Energy Procedia* 7(2011) 589-596

3. A Survey of Genetic Algorithm Applications in Nuclear Fuel Management M.L. Jayalal, S.A.V. SatyaMurty, M. Sai Baba *Journal of Nuclear Engineering and Technology* 4(2014) 45-62

4. Application of Genetic Algorithm Methodologies in Fuel Bundle Burnup Optimization of Pressurized Heavy Water Reactor M.L. Jayalal, Suja Ramachandran, S. Rathakrishnan, S.A.V. SatyaMurty, M. Sai Baba *Nuclear Engineering and Design,* 281 (2015) 58–71

Conferences

1. Application of Genetic Algorithms in Data Mining and Knowledge Acquisition
M.L.Jayalal,S.Rajeswari, S.A.V.SatyaMurty *8th biennial national conference on Recent Advances in Information Technology (READIT-2011)* held at IGCAR, Kalpakkam (2011)

2. Knowledge Discovery Using Genetic Algorithm: A Study M.L.Jayalal, M. Sai Baba, S.Rajeswari, K.K. Kuriakose, S.A.V.SatyaMurty *9th biennial national conference on Recent Advances in Information Technology (READIT-2013)* held at IGCAR, Kalpakkam (2013)

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41. Name : **Debabrata Saha**
Enrolment No. : PHYS03201004014
Date of Award of degree : 27.05.16
Constituent Institute : Raja Ramanna Centre for Advanced Technology,
Title : Effect of Doping on Carrier Transport in ZnO Thin Films Grown by Atomic Layer Deposition.

Abstract

The main aim of the thesis is to study the effect of doping on the temperature dependentelectron transport in intrinsically and/or extrinsically doped ZnO thin film grown by atomiclayer deposition (ALD). Initially, we have optimized various process parameters to grow intrinsic ZnO thin films on (0001) sapphire substrates with optimal structural, optical and electrical properties. The self-limiting growth window for the layer-by-layer growth of intrinsic ZnO thin films was achieved in the temperature range of ~ 140-2000C with a constant growth rate of ~ 0.2 nm/cycle. The crystalline and compositional defects in these films were found to be strongly dependent on growth temperature which significantly influenced the underlying electron transport properties in these films. In order to further increase the n-type conductivity in ZnO films, we have incorporated Al dopants in ZnO through sub-saturating exposure of dopant precursor molecules on the growing film surface. Highly conducting Al doped ZnO (AZO) thin films with a minimum value of room

temperature electrical resistivity ~ 8.6x10-4 Ω cm and comparatively good Hall mobility ~18 cm2/Vs was achieved at ~2.2 at% of Al incorporation. With further increase in Al concentration, a crossover from good metallic to barely metallic resistivity behavior was observed at ~5.5 at% of Al. Presence of disorder induced weak localization and electronelectron interactions due to the diffusive motion of electrons was observed in the temperature dependent electrical resistivity which was further confirmed by magnetoresistance (MR) measurements (5-300 K) in magnetic field of (0-8 T) applied perpendicular to the film surface. Afterward, we have used group IV element Ti as another n-type dopant in ZnO. Ti doped ZnO thin films (TZO) with enhanced doping efficiencies were achieved through in-situ vertical stacking of multiple sub-monolayers of TiOx in ZnO lattice. The degree of static disorder in these films has been tuned in a wide range from good metallic to an incipient nonmetallic regime by varying the period of vertically stacked TiOx sub-monolayers. Electron transport in these films was found to be driven by the intricate interplay of screening and disorder. The temperature dependence of phase-coherence length, as extracted from the MR measurements, indicated inelastic electron-electron scattering as the dominant dephasing mechanism in these dirty metallic systems. Finally we have correlated the optical and electrical properties of these heavily degenerate TZO films. The temperature dependent photoluminescence and room temperature optical absorption spectra were found to be in good conformity with the combined effects of Burstein-Moss band filling and band gap narrowing above Mott critical density of ZnO.

Publications

Journal

1. D. Saha, V. K. Sahu, Amit K. Das, R. S. Ajimsha, P. Misra, L. M. Kukreja,"Studies onoptical and electrical characteristics of ZnO thin films grown by atomic layer deposition",Phys. Express (2013) 3:9 (available at http://www.cognizure.com/abs/106637273.aspx).

2. D. Saha, Amit. K. Das, R. S. Ajimsha, P. Misra, and L. M. Kukreja, "Effect of disorder oncarrier transport in ZnO thin films grown by atomic layer deposition at different temperatures", J. App. Phys. 114, 043703 (2013), (DOI: http://dx.doi.org/10.1063/1.4815941).

3. D. Saha, R.S. Ajimsha, K. Rajiv, C. Mukherjee, M. Gupta, P. Misra, L.M. Kukreja,"Spectroscopic ellipsometry characterization of amorphous and crystallineTiO2 thin filmsgrown by atomic layer deposition at different temperatures", App. Surf. Sci. 315, 116 (2014), (DOI: http://dx.doi.org/10.1016/j.apsusc.2014.07.098).

5. D. Saha, P. Misra, R. S. Ajimsha, M. P. Joshi, and L. M. Kukreja, "Phase coherent transportin (Zn, Al)Ox thin films grown by atomic layer deposition", App. Phys. Lett. 105, 212102(2014), (DOI: http://dx.doi.org/10.1063/1.4902513).

6. D. Saha, P. Misra, M. P. Joshi, and L. M. Kukreja, "Observation of dopant-Profileindependent electron transport in sub-monolayer TiOx stacked ZnO thin films grown byatomic layer deposition", Appl. Phys. Lett. 108, 032101 (2016), (DOI:http://dx.doi.org/10.1063/1.4939926).

7. D. Saha, P. Misra, S. Bhartiya, M. Gupta, M. P. Joshi, and L. M. Kukreja, "Dimensional crossover of electron weak localization in ZnO/TiOx stacked layers grown by atomic layerdeposition", Appl. Phys. Lett. 108, 042109 (2016), (DOI:http://dx.doi.org/10.1063/1.4940977).

8. D. Saha, P. Misra, M. P. Joshi, and L. M. Kukreja, “UV light induced insulator-metaltransition in ultra-thin ZnO/TiOx stacked layer grown by atomic layer deposition”, (under review).

9. D. Saha, P. Misra, M. P. Joshi, and L. M. Kukreja, “Temperature dependent photoluminescence characteristics of atomic layer deposited (Zn, Ti)Ox thin films above Mott’s critical density”, (to be submitted)

Conferences and Workshops:

1. “Structural, optical and electrical properties of intrinsic ZnO thin films grown by atomiclayer deposition” D. Saha, V. K. Sahu, Amit K. Das, R. S. Ajimsha, P. Misra, L. M. Kukreja,DAE-BRNS 6th National Symposium on Pulsed Laser Deposition of Thin Films and Nanostructured Materials (PLD-2011)”, IISc (MRC), Bangalore, November 09-11, 2011.

2. “INUP Familiarization Workshop on Nanofabrication Technologies”, Centre for Nanoscience and Engineering, IISc, Bangalore, January 28-30, 2015.

3. “Hands on Training on MOS Capacitor and Micro and Nano Characterization techniques”, Centre for Nanoscience and Engineering, IISc, Bangalore, 10-19 March 2015.

4. “Temperature Dependent Electron Transport in Degenerately Doped ZnO Thin FilmsGrown by Atomic Layer Deposition”, D. Saha, P. Misra, M. P. Joshi, and L. M. Kukreja,ICMAT, Singapore, 28th June-3rd July 2015.

5. “Dimensional crossover of electron transport in (Zn, Ti)O_x thin films grown by atomiclayer deposition”, D. Saha, P. Misra, M. P. Joshi, and L. M. Kukreja, IWPSD, IISc,Bangalore, 7-10 December 2015.

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42. Name : **Akansha Singh**
Enrolment No. : PHYS08200904001
Date of Award of degree : 07.06.16
Constituent Institute : Harish-Chandra Research Institute
Title : First-Principles Studies Of Subsrate Supported Metal Clusters: From Fundamentals To Applications.

Abstract

Atomic clusters are aggregates of atoms consisting of a few to a few hundred atoms, which exhibit extreme size dependence of properties, which are distinct from those of an atom and corresponding bulk. Some clusters can mimic the properties of elemental atoms and retain their identity in assemblies are termed as superatoms. For these clusters and superatoms to be useful in practical applications, it is essential to support them on some substrate. Cluster arrays and cluster assembled films fabricated over substrates can have applications in electronics and magnetic storage devices. In this thesis we discussed the electronic and structural changes in the clusters after deposition on the surfaces. We analyzed the electronic, magnetic, and catalytic properties of the substrate supported clusters and discuss their potential use in various applications.The first part of thesis consist the results of adsorption of small silver clusters (n = 1-8) on clean graphite using different methods that take dispersive interactions into account and compare them with the experimental results. The ground state structures of Ag_n clusters (n = 1-8) in gas phase and supported over graphite substrate obtained within vdW-DF2 method are discussed. We also argue that the results obtained with vdW-DF2 method are in best agreement with the experimental observation. In the second part, the results of adsorption and diffusion of small silver clusters on a stepped graphite surface are discussed. In their ground state, clusters distort away from symmetric structures in order to maximize the bonding with the step-sites. At finite temperatures clusters break up and the silver atoms start diffusing along the step edge. It has been argued that by controlling the cluster density to match the available step-edge active sites, it may be possible to fabricate self-assembled atomically thin nano-wires. The third part has illustrated the possible support for the magnetic superatom assemblies. Superatoms hold promise to serve as building blocks of nanoscale designer materials. We deposit $FeCa_8$ over different substrates and find that it has strong interactions with α-(0001)Al_2O_3 and calcium(001) surface. We also discuss the behavior of $FeCa_8$ over h-BN and graphene sheet and examine the exchange interactions between two units of $FeCa_8$ over these substrates. The consequences of the magnetic interaction between the supported superatoms have also been discussed. The tentative cluster density to fabricate magnetic cluster assembled films has also been estimated. The last part of the thesis discusses the reactivity of Ag_nAu_m (n + m = 2 - 4) clusters supported over the α-(0001)Al_2O_3 substrate towards CO-oxidation. We described the ground state structures for gas phase Ag_nAu_m (n + m = 2 - 4) clusters and discussed the results for adsorption and coadsorption of CO and O_2 molecules on these clusters. Later we discussed the role of the alumina surface in the CO-oxidations on these clusters and proposed that $AgAu_2$, Ag_2Au and $AgAu_3$ clusters supported over alumina could be the better catalysts for CO-oxidation reaction. We end this thesis with our conclusions and with the discussion of possible future works.

Publications

Journal

1. "Structural, electronic and magnetic properties of binary transition metal aluminum clusters: absence of electronic shell structure", Vikas Chauhan, Akansha Singh, Chiranjib Majumder and Prasenjit Sen, J. Phys. Cond. Matt., 2014, 26, 035438.
2. "Do Ag_n (up to n = 8) clusters retain their identity on graphite? Insights from first-principles calculations including dispersion interactions", Akansha Singh, Chiranjib Majumder and Prasenjit Sen, J. Chem. Phys., 2014, 140, 164705.
3. "Density functional study of silver clusters on a stepped graphite surface: Formation of self-assembled nano-wires", Akansha Singh and Prasenjit Sen, Phys. Chem. Chem. Phys., 2015, 17, 12708.
4. "Finding the right support for magnetic superatom assembly", Akansha Singh and Prasenjit Sen, Phys. Rev. B, 2015, 91, 035438.
5. "Antiferromagnetic spin structure and negative thermal expansion of $Li_2Ni(WO_4)_2$", Sunil K. Karna, C. W. Wang, R. Sankar, M. Avdeev, Akansha Singh, I. Panneer Muthuselvam, V. N. Singh, G. Y. Guo, and F. C. Chou, Phys. Rev. B, 2015, 92, 014413.

Other Publications:

1. "Peierls transition and edge reconstruction in phosphorene nanoribbons", Ajanta Maity, Akansha Singh and Prasenjit Sen, arXiv: 1404.2469 (2014).
2. "A comparative studies of Silver cluster supported over graphite surface using van der Waals interactions", Akansha Singh and Prasenjit Sen, in preparation.
3. Tellurium-bridged two-leg spin ladder in Ba_2CuTeO_6", G. Narsinga Rao, R. Shankar, Akansha Singh, I. Panneer Muthuselvam, Viveka Nand Singh, Guang-Yu Guo and F. C. Chou, Phys. Rev. B, 2016, 93, 10440-104411.
4. "CO-oxidation by α(0001)-Al_2O_3 supported Ag_nAu_m (n+m=2-4) clusters", Akansha Singh, Chiranjib Majumder and Prasenjit Sen, in preparation.

43. Name : **T.L. Prasad**
Enrolment No. : ENGG01200704015
Date of Award of degree : 07.06.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Study Of Recovery Of Heavy Metal Ions From Seawater By Novel Adsorbents

Abstract

Selective separation of valuable heavy metals from lean sources such as seawater/brine is an area of considerable interest for recovering these metals from the vast secondary resources. Various novel techniques are being attempted by researchers for efficient and economical way of recovering these metals [1]. General reagents or sorbents such as bi-functional ion selective polymer supported reagents; biosorbents; functionalised organic ceramic sorbents; polymeric ligand exchangers; molecular imprinting polymers; solvent impregnated resins and grafted sorbents are some of the suggested choices [2-6]. The concentration of uranium in seawater is at least three orders of magnitude less than the conventional primary resources, which are fast depleting. Hence a method, which evolved in the recent past, is the use of adsorbent for recovery of uranium from seawater. And the adsorbent should have superior property with respect to selective adsorption and regeneration. “Radiation grafting on polymers” facilitates for imparting of superior properties onto polymeric adsorbents [7-10]. The parametric sensitivity analysis of such radiation grafting and the use of resultant polymeric adsorbent for recovering the uranium are investigated in this thesis [11]. Grafting is used in situations where the requirements for bulk and surface properties cannot be readily created by using single polymeric material [12-14]. Radiation grafting has made it possible to create a material whose bulk is made of one polymer type but with a surface of another polymer type. A chemical bond is formed between the grafted moiety and the bulk material. During irradiation of polymers free radicals are produced in the material without the use of chemicals. Any amount of functional groups can be introduced to the trunk polymer fiber by selecting proper type of irradiation and grafting conditions. Electron beam irradiation eliminates the sensitivity of catalysts to temperature. An efficient grafting technique needs to be developed to reduce the manufacturing cost of radiation grafted polymeric adsorbents. Higher selectivity and more efficient adsorption properties can be imparted with proper selection of ligand and by controlling the functionality of grafted chains. Considering a large number of parameters and variables in radiation grafting, results have been reported in this research work [15]. Studies on radiation grafting polymerization of monomers to monofilament fibers and systematic evaluation of grafting conditions for an optimum grafting yield have been reported, with a view for recovery of heavy metals such as uranium and vanadium. In this thesis, each aspect of radiation grafting and application stages to establish metal pick up characteristics have been presented for variety of polymeric substrate materials.

Publications

Journal

1. Prasad, T.L., Saxena, A.K., Tewari, P.K., Sathiyamoorthy, D., (2009) “An Engineering Scale Study on Radiation grafting of polymeric adsorbents for recovery of Heavy Metal Ions from Seawater ”, Nuclear Engineering and Technology, Vol 41, No.8, pp 1101-1108
2. Prasad, NK, Pathak,K, Kumar, M, Matkar, AW, Prasad, TL and Saxena, AK (2009) “Challenges in the design of a prototype contactor assembly for the recovery of uranium from seawater”, Int Jounal of Nuclear Desalination, Vol 3, No.3, pp241-246

3. Prasad, T.L., Tewari, P.K., Sathiyamoorthy, D., (2010) “Parametric studies on radiation grafting of polymeric sorbent for recovery of heavy metals from seawater”, Ind. Eng. Chem. Res, Vol 49, pp 6559-6565
4. Prasad, T.L., Tewari, P.K., Sathiyamoorthy, D., (2011) “Sorption kinetic studies using metal chelate embedded polymers for recovery of heavy metals from desalination effluents r”, International Journal of Nuclear Desalination, Vol 4, No. 3, pp 261-276b) Accepted 01
5. Reviewer-1 comments are received for JRNC (special issue of Journal of Radiation and Nuclear Chemistry) manuscript.

Other Conferences:

1. Prasad TL., Tewari PK., Sathiyamoorthy D., “Recovery of uranium from reject streams of Desalination plants” was presented at Eighteenth annual conference of Indian Nuclear Society held at Nuclear Fuel Complex Hyderabad during November 21-24, 2007.
2. Prasad TL Tewari PK “Recovery of Uranium and other valuables from Seawater/Brine” was made under Indo French Collaboration on Integrated Nuclear Desalination Systems during 3rd Technical meeting at BARC (Trombay) India on 3rd March, 2008.
3. Prasad, T.L., Tewari, P.K., Sathiyamoorthy D., Kalsi, P.C., Acharya, R., Manchanda, V.K., “ Advanced Techniques for measurement of heavy metal concentrations from seawater “ Presented at International conference 62nd Indian Chemical Engineering congress CHEMCON-2009, Organised by Indian Institute of Chemical Engineers in association with Waltair Regional Centre held at Andhra University Vishakapatnam, December 27-30, 2009
4. Prasad, T.L., Tewari, P.K., Sathiyamoorthy D., Kalsi, P.C., Acharya, R., Manchanda, V.K., “ Nuclear Analytical Techniques for Recovery of uranium from seawater “ Presented at Fourth International symposium NAC-IV Cosponsored by Board of Research in Nuclear Sciences held at Bhabha Atomic Research Centre Mumbai, November 15-19, 2010.

5. Prasad, T.L., Prasad, N.K., Tewari, P.K., Sathiyamoorthy D., “ Technology to harvest uranium from sea – Development studies on Radiation grafting reactor systems “ Presented at International conference 63rd Indian Chemical Engineering congress CHEMCON-2010, Organised by Indian Institute of Chemical Engineers in association with Neyveli Regional Centre held at Annamalai University Chidambaram, December 27-29, 2010
6. Prasad, T.L., Tewari, P.K., “ Radiation grafted polymeric sorbents for Recovery of uranium from Desalination effluents “ Presented at Indo-UK workshop-2011 on Current development of wastewater treatment in India, Organised by National Institute Technology Tiruchy and supported by Royal Society UK and Department of Science and Technology, held at Tiruchy, August 29-31, 2011

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44. Name : **Sabyasachi Tarat**
Enrolment No. : PHYS08200804004
Date of Award of degree : 07.06.16
Constituent Institute : Harish-Chandra Research Institute
Title : Thermal fluctuations in disordered superconductors.

Abstract

The predictions of BCS theory need to be modified for (a) strong interaction between electrons, (b) the presence of significant potential scattering, leading to a superconductor-insulator transition (SIT), (c) the coupling to magnetic impurities, and, for example, (d) the proximity to other ordered phases. As a result, we

need to handle inhomogeneous ground states and quantum and thermal fluctuations of the 'order parameter'. Our primary focus is on understanding the role of strong disorder in superconducting systems, in particular the thermal fluctuation effects that occur on the inhomogeneous background.

- After providing summaries of the experimental, theoretical and numerical work done on disordered superconductors, we introduce our auxiliary field model and discuss in detail how we solve it using numerical Monte Carlo and extract observables from it. We then apply it to the BCS-BEC crossover in 2D to benchmark our model. Our approach leads to a Tc scale that agrees with quantum Monte Carlo. We discuss results on the Tc, amplitude and phase fluctuations, density of states, and the momentum resolved spectral function, over the entire interaction and temperature window and compare them with full QMC and other semi-analytic approaches.

- We then analyze the disorder driven SIT at finite temperature. We track the Tc, the resistivity, the global density of states (DOS) and the optical conductivity with increasing disorder. Beyond moderate disorder the low temperature superconducting state arises out of an 'insulating' normal state. A disorder driven deepening pseudogap in DOS and a divergence of the Tc and the gap vanishing temperature at strong disorder is seen. We find low frequency weight in the density of states and optical conductivity are non-monotonic in disorder. We compare our results to recent experimental data.

- Next, we move to local properties. We discuss how the disorder landscape generates inhomogeneities. We study the spatially differentiated amplitude and phase fluctuations in this background and establish spatial maps of the coherence peak as the superconductor is driven through the thermal transition. Local density of states reveals that superconducting regions shrink and fragment with increasing temperature, but survive in small clusters to a temperature Tclust>> Tc. The gap (or pseudogap) in the spectrum survives to another independent scale, Tg. We discuss the physical origin of these multiple scales, suggest a Ginzburg-Landau scheme to describe the situation, and compare our results in detail with experiments.

- We then investigate the effect of magnetic impurities on superconductivity at fixed interaction strength for various impurity spin coupling J. We present phase diagrams showing the gapped, gapless and non-superconducting phases in the J-T window, and analyze their dependence on J. We provide detailed results on the density of states showing the formation of subgap impurity levels. Our results reveal that the gapless phase increases in size with increasing J. Additionally, we find that at large J, the lowest energy wavefunctions are concentrated near the impurity positions, which also act as nucleation centres for the loss of SC with increasing temperature.

Publications

Journal

1. "Pairing fluctuations, the BCS-BEC crossover and strong disorder in superconductors ",Pinaki Majumdar and SabyasachiTarat, Journal of Superconductivity and Novel Magnetism, 2013, Vol. 26, 1787-1793.
2. "Charge dynamics across the disorder driven superconductor-insulator transition ,Sabyasachi Tarat and PinakiMajumdar,Europhysics Letters, 2014, Vol. 105, 67002p1-67002p6.
3. "A real space auxiliary field approach to the BCS-BE crossover ", Sabyasachi TaratandPinakiMajumdar, European Physical Journal B, 2015, Vol. 88, 1-10.

4. “Tunneling spectroscopy across the superconductor-insulator thermal transition”,SabyasachiTarat and PinakiMajumdar, arXiv:1406.5423, 2014.
5. “Dense magnetic impurities in a s-wave superconductor: thermal and strong couplingeffects beyond Abrikosov-Gorkov theory” (in preparation), Sabyasachi Tarat and PinakiMajumdar.

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45. Name : **Sunil Tonpe**
Enrolment No. : ENGG02200804021
Date of Award of degree : 08.06.16
Constituent Institute : Indira Gandhi Centre for Atomic Research
Title : Microstructure-Corrosion Correlation Studies On Thermo-Mechanically Process3ed Zirconium Based Alloys.

Abstract

Zirconium based alloys are the main choice for both fuel clad, and in-core structural components of the water cooled thermal reactors. For the fast breeder reactor (FBR) spent nuclear fuel reprocessing plants, zirconium-based alloys are considered as a candidate dissolver material for its high corrosion resistance. As for examples, the Zr-2, Zr-4, Zr-1%Nb, Zr-2.5%Nb and Zr-2.5%Nb-O.5%Cu are the well-known alloys developed for structural and fuel cladding applications in the nuclear reactor. Mock up dissolver vessel made of Zr-4 has been fabricated for reprocessing fuel form FBR. In the present work, the microstructural, mechanical properties and corrosion behavior investigations were carried out on various zirconium based alloys under various thermo-mechanical processes. Characterization techniques like OM, SEM, SEM-EDS and XRD have been used in the present study to optimize the desired microstructure. Tensile testing and Vickers hardness measurements were used for the evaluation of mechanical properties like yield strength (YS), ultimate tensile strength (UTS) and micro-hardness at room temperature. Corrosion behaviors of such processed zirconium, Zr-2, Zr-4, Zr-1%Nb and Zr-2.5%Nb alloys were evaluated in boiling 11.5 M nitric acid (i.e., ASTM A262 Practice C test) to evaluate their corrosion resistance and correlate with the microstructure and passive oxide layers (characterized by LRS and XPS) after various processing steps. In zirconium alloys of Zr-2.5% Nb and Zr-1% Nb alloy, the microstructure consists of the of fast cooled martensitic parallel plate morphology. The Zr-2.5%Nb and Zr-1% Nb alloys consist of primary phase as a α-Zirconium (hcp) and secondary phase as β-Zirconium (bcc). Cast ingot shows low mechanical properties and hardness with considerable percentage elongation. Low mechanical properties can be attributed to coarse dendritic cast grain structure. TIG welded Zr-4 exhibited a hardness value of 387VHN while the hardness of the base metal observed at 183VHN, and EB weld showed 197VHN. The increase in the hardness in the TIG weld region is due to increase in oxygen or nitrogen value. Thereby, mechanical properties depend strongly on the composition of the zirconium alloys and thermo-mechanical processing conditions.The corrosion rate obtained in boiling 11.5 M HNO_3 as per ASTM A262 Practice C for 240 h for tube Zr-2, Zr-4, Zr-2.5%Nb and Zr-1%Nb are 0.04, 0.02, 0.08 and 0.07 respectively and for autoclaved Zr-4 tube is 0.003 mpy. Similarly, the corrosion rate of long-term corrosion loop test for as-cast ingots of unalloyed zirconium, Zr-2, Zr-4 and Zr-1%Nb are 0.005, 0.006, 0.006 and 0.006 mpy respectively and for as-cast Zr-2.5%Nb ingot is 0.15 mpy. In summary, insignificant corrosion rate was observed between different grades of zirconium in boiling nitric acid and the corrosion rate is unaffected by the metallurgical state. Since the corrosion of zirconium is negligible, no maintenance and inspection may not be required for a radioactive environment, and extended plant component life can be realized.

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2. Sunil Tonpe, N. Saibaba, R.N. Jayaraj, A. Ravi Kumar, U. Kamachi Mudali, Baldev Raj, Process development for fabrication of zircaloy-4 dissolver assembly for reprocessing of spent nuclear fuel, Energy Procedia 7 (2011) 459-467.
3. V. Deshmukh, Uppal Singha, Sunil Tonpe, N. Saibaba, Effect of process variables on texture and creep of preessurized heavy water reactor pressure tube, Transactions. IIM, 63 (2010) 397-402.

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2. Sunil Tonpe, A. M. Parsodkar, C.M. Prabhu, N. Saibaba Fabrication of reactivity control assemblies for 540 MWe PHWR, ibid.
3. Sunil Tonpe, Uppal Singha, V. Deshmukh, N. Saibaba, Fabrication of seamless pressure tubes and calandria tubes for PHWR through pilgering route, ibid.
4. V. Deshmukh, Kumar Vaibhav, SK Jha, Sunil Tonpe, N. Saibaba, Development of heat treated Zr-2.5Nb pressure tubes, ibid.
5. S. Srinivaslu Reddy, Sunil Tonpe, N. Saibaba, Optimization of process parameters for control of hydrogen in garter springs for PHWRs, HEM, BARC, Mumbai, 2008.
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7. Sunil Tonpe, Uppal Singha, V. Deshmukh, N. Saibaba, Hexagonal channel by seamless pilger route for Prototype fast breeder reactor, INSAC-2009, Chennai.
8. M. Kamesh, Sunil Tonpe, N. Saibaba, R.N. Jayaraj Manufacture of components for PHWR& BWR fuel bundles, ibid.
9. Uppal Singha, V. Deshmukh, Sunil Tonpe, N. Saibaba, Process development for manufacturing of square channels through seamless pilgering route, ibid.
10. V. Deshmukh, Sunil Tonpe, Uppal Singha, N. Saibaba , Development of heat treated Zr-2.5Nb pressure tubes, ibid.
11. V. Deshmukh, Uppal Singha, Sunil Tonpe, N. Saibaba and R. N. Jayaraj, Manufacture of Zirconium Alloy Square Channels for BWRs through Pilger Route, ibid, R-35, P. 220.
12. V. Deshmukh, K. Vaibhaw, S.K. Jha, Sunil Tonpe and N. Saibaba, Development of Zr-2.5% Nb Pressure Tubes through Heat Treated Route, In: Proceeding International Conference on Peaceful Uses of Atomic Energy-2009, September 29 - October 1, 2009, Vigyan Bhavan, New Delhi, Editors: A.V.R. Reddy, V. Venugopal, R. K. Sinha, S. Banerjee, Vol. 1. R-26, P. 202.
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15. V. Deshmukh, Sunil Tonpe, Uppal Singha, N. Saibaba, Effect of process variables on texture and creep of PHWR pressure tubes, Kalpakkam CF-8, 2010.
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Report

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46. Name : **Kedar Narsinha Yogi**
Enrolment No. : LIFE09200904006
Date of Award of degree : 08.06.16
Constituent Institute : Tata Memorial Centre
Title : WNT signalling driven up-regulation of microRNAs in medulloblastoma

Abstract

Medulloblastoma is classified in four distinct molecular subgroups viz. WNT, SHH, Group 3 and Group 4. These subgroups also differ in their microRNA profile with the WNT subgroup tumors having the most distinctive microRNA profile with a number of microRNA upregulated in the WNT subgroup as compared to other subgroups as well as normal cerebellum. The present study was undertaken in order to understand whether transcription WNT subgroup specific miRNAs viz. miR-193a, miR-148a, miR-365 and miR-224 is directly or indirectly regulated by WNT signaling pathway. Further the role of miR-148a in modulating proliferative, migratory and tumorigenic potential of medulloblastoma cells was also investigated. Activity of both miR-148a and miR-193a promoter was found to be induced upon expression of MYC, a known target of the WNT signaling pathway. Bisulfite sequencing of MiR-148a promoter region showed hypermethylation of CpG island in non-WNT medulloblastoms and in established Group 3 medulloblastoma cell lines. Treatment with HDAC inhibitor was shown to bring about upregulation of miR-148a expression in a medulloblastoma cell line. Thus, MiR-148a expression in WNT subgroup medulloblastomas appears to be induced by MYC expression while its expression is suppressed in non-WNT medulloblastomas as a result of epigenetic modifications. MiR-148a was expressed in non-WNT medulloblastoma cell lines at levels comparable to that in the WNT tumors using inducible lentiviral vectors. MiR-148a expression was found to inhibit growth and bring about reduction in the clonogenic potential, invasion potential and tumorigenicity of medulloblastoma cells. Neuropilin 1 was identified as a novel miR- 148a target gene in medulloblastoma. MiR-148a mediated inhibition in invasion potential and *in vivo* tumorigenicity of medulloblastoma cells was restored upon NRP1 expression, indicating the importance of NRP1 as a key miR-148a target gene in medulloblastoma. Furthermore, NRP1 expression in medulloblastomas was found to be associated with poor survival, with little or no expression in majority of the WNT tumors, indicating its usefulness as marker for prognostication. The tumor suppressive effect of miR-148a expression accompanied by the down-regulation of NRP1 makes miR-148a an attractive therapeutic agent for the treatment of medulloblastomas.

Publications

Journal

MiR-148a, a microRNA upregulated in the WNT subgroup tumors, inhibits invasion and tumorigenic potential of medulloblastoma cells by targeting Neuropilin1 Kedar Yogi, Epari Sridhar, Naina Goel, Rakesh Jalali, Atul Goel, Ali Asgar Moiyadi, Rahul Thorat, Pooja Panwalkar, Atul Khire, Archya Daspgupta, Prakash Shetty, and Neelam Vishwanath Shirsat, Oncoscience. 2015 Mar 2;2(4):334-48. eCollection 2015. PMID: 26097868

Conferences:

1. Participated and presented abstract titled 'Role of miR-148a up-regulated in WNT subgroup medulloblastomas' as a poster presentation at XXXVI All India Cell Biology Conference and International Symposium on "Stress Adaptive Response and Genome Integrity (SARGI) held on 17-19th October 2012 at Bhabha Atomic Research Centre (BARC), Mumbai
2. Participated and presented abstract titled 'Role of miR-148a in WNT subgroup Medulloblastoma' as an oral presentation at 9th National Research Scholars Meet in Life Sciences (NRSM) held at Advanced Centre for Treatment, Research and Education in Cancer (ACTREC) on 18-19th December 2014
3. Participated and presented abstract titled 'miR-148a functions as tumour-suppressor microRNA in medulloblastoma cell lines by targeting Neuropilin1', as a poster presentation at AACR special series conference "Advances in Brain Cancer Research held on 27-30th May 2015 at Washington D.C.

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47. Name : **B. Ravinder**
Enrolment No. : MATH10200904003
Date of Award of degree : 13.06.16
Constituent Institute : Institute of Mathematical Sciences,
Title : On bases for local Weyl modules in type A.

Abstract

This thesis is a study of the Chari-Pressley-Loktev (CPL) bases for local Weyl modules of the current algebra associated to a special linear Lie algebra. As convenient parametrizing sets of these bases, we introduce the notion of partition overlaid patterns (POPs), which play a role analogous to that played by (Gelfand-Tsetlin) patterns in the representation theory of the special linear Lie algebra. The notion of a POP leads naturally to the notion of area of a pattern. We observe that there is a unique pattern of maximal area among all those with a given bounding sequence and given weight. We give a combinatorial proof of this and discuss its representation theoretic relevance. We prove the \stability", i.e., compatibility in the long range, of CPL bases with respect to inclusions of local Weyl modules in the rank one case and state it as a conjecture for higher rank cases. In order to state the conjecture, we establish a certain bijection between colored partitions and POPs, which is of interest in itself. Irreducible representations of the special linear Lie algebra occur as gradeb zero pieces of the corresponding local Weyl modules. The CPL basis being homogeneous, those basis elements that are of grade zero form a basis for the irreducible representation space. We prove a triangular relationship between this basis and the classical Gelfand-Tsetlin basis.

Publications

Journal

1. Stability of the Chari-Pressley-Loktev bases for local Weyl modules of sl2[t]", K. N. Raghavan, B. Ravinder, S. Viswanath, Algebr. Represent. Theory 18 (2015), no. 3, 613{632.

Preprints

1. On Chari-Loktev bases for localWeyl modules in type A", K. N. Ragha-van, B. Ravinder, S. Viswanath, (2016).

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48. Name : **Mahendra Chinthala**
Enrolment No. : ENGG02201004009
Date of Award of degree : 13.06.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Separation Of Cesium From Simulated High Level Waste Using Electrodialysis Ion Exchange.

Abstract

Cs-137 being radioactive in nature finds application in sterilization of medical accessories, food preservation, brachytherapy, blood irradiation, hygienization of sewage sludge etc. Owing to its several medical and industrial applications, separation of Cs from nuclear waste in pure form would be a potential step. Ammonium molybdophospahte Polyacrylonitrile (AMP-PAN) has been extensively studied for selective uptake of Cs from acidic solutions. Regeneration of AMP-PAN should be done with high concentration of eluant (ammonium salt solution) to recover sorbed cesium. Recovery of Cs in pure and concentrated state from high concentrated ammonium solution requires further operations with other ion exchange materials or other methods. Simulated waste containing Cs was passed through a bed of AMP-PAN ion exchange resin packed in a glass column. Various parameters affecting the sorption process like feed flow rate, initial concentration and bed height were studied and the sorption kinetics were predicted using the mathematical models. A hybrid process combining Electrodialysis Ion exchange (EDIX) has been investigated for the recovery of Cs from Cs sorbed AMP-PAN in pure and concentrated form with limited number of operations. The electrodialysis cell was operated in two different modes for the recovery of Cs from AMP-PAN. In mode-I, eluant (ammonium sulphate) is passed as anolyte and in mode-II, eluant is passed directly through the ion exchange resin in the middle compartment of the electrodialysis cell. In both modes of operation, eluant ($(NH_4)_2SO_4$) containing NH_4^+ migrates on application of electric potential towards cathode. Since cathode is negatively charged, it attracts positive charged ions only. On its way towards cathode, NH_4^+ ions replace sorbed Cs^+ on AMP-PAN and the exchanged Cs^+ is available for migration towards cathode. Thus Cs on the AMP-PAN is recovered and concentrated in cathode compartment by application of electric potential. Some ammonium was also migrating along with Cs towards cathode which will convert to ammonia gas form due the generation of hydroxyl ions at the cathode surface. Thus pure Cs can be obtained by EDIX in limited number of operations.Effects of different parameters like current' density, eluant concentration were studied in both modes of operation. By this process, 80% of Cs could be recovered in pure and concentrated form. Current density and eluant concentration played a significant role in the recovery of Cs from AMP-PAN and both were optimized by studying the concentration polarization effect in the electrodialysis cell. An empirical equation was proposed for the determination of limiting current density below which the cell should be operated. Operation of the cell at 80 % of the limiting current density was suggested.

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2. Ch. Mahendra, P.M. Satya Sai, C. Anand Babu, Current -Voltage characteristics in EDIX for separation of cesium from AMP-PAN. Desalination 353 (2014) 8-14.
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2. Ch.Mahendra, P.M. Satya Sai, C. Anand Babu, K.Revathy, K.K.Rajan, Application of Thomas Model for ion exchange of cesium on AMP-PAN, International Conference on Chemical and Bioprocess Engineering, NITW, Warangal, Nov 23, 2013.
3. Ch.Mahendra, P.M. Satya Sai, C. Anand Babu, K.Revathy, K.K.Rajan, Electrodeionization of cesium from AMP-PAN, CHEMCON13, ICT, Mumbai, Dec 27, 2013.
4. Ch.Mahendra, P.M. Satya Sai, C. Anand Babu, K.Revathy, K.K.Rajan, Intergration of Ion exchange and Electrodialysis for the separation of cesium form simulated High Level Waste, Interenational Conference on Innovative Technologies and Management for Water Security, NIOT, Chennai, Feb 12, 2014.
5. Ch.Mahendra, P.M. Satya Sai, C. Anand Babu, K.Revathy, K.K.Rajan, Effect of electrolytes concentration on recovery of cesium from AMP-PAN by Electrodialysis- Ion exchange (EDIX), SESTEC 14, BARC, Mumbai, Feb 25-28, 2014.

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49.			
	Name	:	**Raja Reddy Kuppili**
	Enrolment No.	:	LIFE09201004009
	Date of Award of degree	:	13.06.16
	Constituent Institute	:	Tata Memorial Centre
	Title	:	Understanding the mechanism of apoptosis regulation involving anti-apoptotic HAXI and pro-apoptotic serine protease HtrA2/Omi.

Abstract

HtrA2, a trimeric proapoptotic serine protease plays pivotal role in maintaining cellular homeostasis by mediating apoptosis via multiple pathways. Differential expression of HtrA2 has been associated with neurodegenerative diseases, hepatocellular carcinoma as well as cancers such as, ovarian, breast and prostatic thus making it an important therapeutic target. Upon substrate binding, this protein regulates its functions through coordinated conformational changes the mechanism of which is yet to be elucidated. Most of its cytoplasmic partners and substrates such as IAPs, Pag, Mxi-2 and Pea-15 [6, 7-8] suggest an interaction after being released from the mitochondria. However, subsequent studies have identified a mitochondrial anti-apoptotic protein HAX1 (Hematopoietic cell specific Lyn-substrate 1) as a binding partner cum substrate of HtrA2, which on interaction with the latter degrades and leads to subsequent activation of

HtrA2 as an early event in apoptosis [9]. However, details of this interacting complex and mechanism of action are yet to be delineated. Although allostery has been found in some of its homologs, it has not been very well characterized in HtrA2. Our *in silico* studies led to prediction of the putative binding pocket which together with modeling, molecular dynamics simulation, enzymology and other biochemical studies helped us identify and demonstrate its role in allosteric regulation of HtrA2 activity. This non-classical binding pocket is unique among HtrA family proteins and thus unfolds a novel mechanism of regulation of HtrA2 activity and hence apoptosis. In the cellular scenario, the allosteric mechanism is of significance for HtrA2 regulation by its binding partners and vice-versa. Hence, the other part of our study was to elucidate the mechanism of intrinsic pathway of apoptosis in context of HtrA2 and one of its key interacting partners in the mitochondria, HAX1. HAX1 is a ubiquitously expressing anti-apoptotic protein that regulates mitochondrial membrane potential. Despite suggestions of their involvement in a novel alternate apoptotic pathway, the structural details, stoichiometry and mechanism of HtrA2-HAX-1 interaction and subsequent event in the mitochondria are yet to be elucidated. Our *in silico* interaction studies and *in vitro* pull down assays have provided information on interacting domains, the minimal binding region and the critical residues involved. With comprehensive enzymology studies we also provide evidence demonstrating for the first time that HAX1 is an activator of HtrA2 which could prove to be a critical step driving early stages of apoptosis. The other players in the complex mechanism were also taken into consideration for better insights in the mechanism. These studies put together have helped us design allosteric peptide modulators that might be an excellent approach to modulate HtrA2 functions. The peptide based approach has been found to exhibit several advantages over conventional orthosteric molecules, such as low toxicity and higher subtype specificity. These findings can thus be utilized for designing small molecule inhibitors in therapeutic strategies against cancer and other diseases. While trying to understand the domain architecture and the roles of different domains in HtrA2, we realized the importance of the PDZ domain both in the functional dynamics of the protein as well as protein-protein interactions. But surprisingly there is not a single database with updated information on this important class of PDZ containing proteins and their interacting partners. With an aim at providing updated and comprehensive information on these proteins, we developed a PDZ domain database, 'PDZome,' that comprises details of 42,043 proteins and their interacting partners. This will be of great value to both basic and clinical researchers in this field both for identifying new targets as well as establishing therapeutic strategies.

Publications

Journal

1. Allosteric regulation of serine protease HtrA2 through novel non-canonical substrate binding pocket. Kuppili R R§, Bejugam P.R§, Singh N, Gadewal N, Chaganti L K, Sastry M, Bose K*. Plos One 2013; 8(2):e55416. doi: 10.1371/journal.pone.0055416. Epub Feb 2013. § (Authors with equal contribution).
2. Intricate structural coordination and domain plasticity regulate activity of serine protease HtrA2. Chaganti LK, Kuppili RR, Bose K. FASEB J. 2013 Aug; 27(8):3054-66. Epub Apr 22, 2013.
3. The structural basis of mode of activation and functional diversity: A case study with HtrA family of serine proteases. Singh N, Kuppili R R, Bose K* (Review article) Archives of Biochemistry and Biophysics. 2011 Dec 15; 516(2):85-96.

Conferences

1. Presented Poster titled 'Delineating the mechanism of HtrA2 mediated HAX1 regulation in the intrinsic pathway of apoptosis' at the Keystone Symposia on "Frontiers of Structural Biology". UT, USA, March 2014.
2. Presented poster titled "Allosteric regulation of pro-apoptotic serine protease HtrA2", at the "International symposium on the Conceptual Advances in cellular homeostasis regulated by proteases and chaperones", ACTREC, Navi Mumbai, India, Dec 2013.
3. Won 2nd prize for Poster & Oral presentation for "Allosteric regulation of pro-apoptotic serine protease HtrA2" at "Accelerating Biology 2013: The Next Wave" organized by C-DAC, Pune, India in Feb 2013.

4. Presented Poster at the Conference on “Recent Advances in Computational Drug Design”, IISC, Bangalore, India in Sep 2013.
5. Presented Poster at the Annual meeting of the Indian Biophysical Society (IBS), held at University of Mumbai, India in Jan 2013.
6. Selected for Oral presentation titled Biophysical characterisation of HAX1, a key player in the intrinsic pathway of apoptosis at the Annual meeting of the Indian Biophysical Society (IBS), University of Madras, Jan 2012.

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50. Name : **B.K. Nashine**
Enrolment No. : ENGG02200804010
Date of Award of degree : 13.06.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Design and Development of Sodium Submersible Electromagnetic Pump for High Temperature Application.

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51. Name : **R.S. Patwardhan**
Enrolment No. : LIFE01201104004
Date of Award of degree : 14.06.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Amelioration of Ionizing Radiation Induced Cell Death in Lymphocytes by Baicalein.

Abstract

Planned or unplanned exposure to Ionizing Radiation (IR) can occur for variety of reasons in human life. Peaceful use of atomic energy for diagnostic and therapeutic purposes, food irradiation, sterilization of medical equipment and sanitary products, sludge treatment, power production and strategic purposes etc is becoming more popular and hence the chances of accidental or occupational exposure have also increased. Presently, our unpreparedness to provide concrete medical countermeasure and inability to cover risk of bulk damage to population has severely compromised risk/benefit ratio for use of IR [1]. IR is known to alter the functions of cellular macro-molecules leading to tissue damage. The deleterious effects of ionizing radiation (IR) are mediated both through the direct deposition of energy to critical biomolecules, and indirectly through the generation of highly reactive free radicals. Approximately 75% of the damage to cells is accounted through indirect effect by low LET ionizing radiations. This cellular damage is manifested through system specific syndromes categorized based on the dose range of exposure. Immune system is vulnerable toIR mediated damage leading to subsequent fatal consequences. Protection or reconstitution of the hematopoietic system is a critical area of research in the development of radioprotectors and therapeutic agents. Exposure of animals to radiation doses above1 Gy leads to hematopoietic syndrome resulting in leucopenia. Hematopoietic recovery after radiation exposure is dependent on the presence of spared hematopoietic stem and progenitor cells in the bone marrow.Currently there are no radioprotectors or mitigators available that are approved by Food and Drug Administration (FDA) for general use in humans for the prevention or treatment of IR induced hematological toxicity. Amifostine (EthyolR) is the only drug approved by the FDA to reduce the toxicity of radiation therapy for limited clinical indications [2]. Recent reports on several phytochemicals have demonstrated their radiomodulatory activity in experimental animal systems. Some of them viz. genestein and gamma tocotrienol analog are at advanced stages of drug development as radioprotector [3, 4]. Some of these potential radioprotective phytochemicals are plant secondary metabolites synthesized by phenylpropanoid pathway that include a variety of plant polyphenols viz., alkaloids, terpenoids, quinones, flavonoids etc. They primarily serve to protect plants against variety of

biotic and abiotic stresses such as UV irradiation, ozone, pollutants, wound, oxidative stress, infection and herbivores. Baicalein, 5,6,7-trihydroxyflavone isolated from dried roots of Chinese herbal medicinal plant *Scutellaria baicalensis*has been shown to inhibit 12-lipoxygenase and it induces apoptosis in several cancer cells such as breast carcinoma cells, colon carcinoma cells, and leukemia cells[5-7]. Baicalein exhibits free radical-scavenging activity and attenuates oxidative stress [8]. Previous studies from our laboratory have demonstrated anti-oxidant and radioprotective properties of baicalein in cell free system. Structurally, it is similar to soy isoflavone geneistein (4, 5, 7-trihydroxyflavone) which is being tested as a radioprotector[9]. In the present study, efficacy of baicalein as a radioprotector and immunomodulator was investigated using mouse model.

Publications

Journal

1. "Involvement of ERK-Nrf-2 signaling in ionizing radiation induced cell death in normal and tumor cells", Patwardhan RS, Checker R, Sharma D, Sandur SK, Sainis KB PLoS One. 2013;8(6):e65929
2. "Mitigation of radiation-induced hematopoietic injury via regulation of cellular MAPK/phosphatase levels and increasing hematopoietic stem cells", Patwardhan RS, Sharma D, Checker R, Sandur SK Free Radical Biology & Medicine 2014;68:52-64
3. "Spatio-Temporal Changes in Glutathione and Thioredoxin Redox Couples during Ionizing Radiation Induced Oxidative Stress Regulate Tumor Radio-resistance", Patwardhan RS, Sharma D, Checker R, Thoh M, Sandur SK Free Radical Research 2015;26:1-15
4. "Baicalein exhibits anti-inflammatory effects via inhibition of NF-κBtransactivation", Raghavendra S. Patwardhan, Deepak Sharma, MaikhoThoh, Rahul Checker, Santosh K. SandurBiochemical Pharmacology2016;108:75–89

Communicated

1. "Baicalein induced cell death in murine T cell lymphoma via inhibition of thioredoxin system" Patwardhan RS, Sharma D, Sandur SK

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52. Name : **Manoj Kumar Tripathy**
Enrolment No. : CHEM01200804021
Date of Award of degree : 14.06.16
Constituent Institute : Bhabha Atomic Research Centre
Title : Theoretical Studies On Molecular Interactions Under Nanoconfinement And Catalytic Properties Of Nanoclusters.

Abstract

The chemical properties of nanomaterials are significantly different from bulk primarily because of the surface induced effect and quantum size effect. The novel properties of nanomaterials make them highly suitable for catalytic and other technological applications. In addition, when the system of nanometer in size is confined in a nanospace environment, the geometric constraint offered by the confinement medium along with the diverse nature of interaction between the enclosed molecules and the medium can drastically modify the physical and chemical properties of the confined system. In the present thesis, structure, energetics, solvation characteristics, vibrational frequencies, chemical reactivity and catalytic activity of nanosystems have been studied using density functional theory based methods. The main objective is to investigate the modification in chemical properties of system by changing the surrounding/local environment.In the first part of the work, the effect of several confinement media such as carbon nanotubes, boron-nitride nanotubes and fullerenes on the molecular properties of water and acid-base complexes have been investigated. The results indicate that the chemical properties of the confined species can be finely modulated by subjecting the species into a proper confinement medium. For instance, it has been shown that the proton transfer in some acid-base pairs, which is not spontaneous in gas phase become possible under the confinement of fullerene by selecting

the appropriate confinement length. In the second part, an analytical expression for the solvation energy for a finite (N) system has been derived using microscopic theory-based bottom-up approach. This approach provides the information on solvation energies of anionic solutes in finite-size clusters, including the bulk ($N = \infty$), from the knowledge of the detachment energies for the system containing a few numbers of solvent molecules. In the last part of the work, catalytic properties of metal atoms and clusters of titanium, vanadiumandgold have been evaluated through a few important reactions such as CO oxidation and water dissociation process. The results indicate that the catalytic activity of metal atoms and clusters can be enhanced by doping with hydrogen atom and by using suitable nanostructured material as substrate.

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Journal

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2. Effect of confinement on the structure and energetics of Zundelcation present inside the hydrophobic carbon nanotubes: An *ab initio* study; M. K. Tripathy, N. K. Jena, A. K. Samanta, S. K. Ghosh, K. R. S. Chandrakumar;Theor. Chem. Acc., 133 (2014) 1576 (1-12).
3. Protonated water under hydrophobic nanoconfinement: An *ab initio* study; M. K. Tripathy, K. R. S.Chandrakumar, and S. K. Ghosh; AIP Conf. Proc., 1512 (2013) 168-169.
4. Water molecule encapsulated in carbon nanotube model systems: Effect of confinement and curvature; N. K. Jena, M. K. Tripathy, A. K. Samanta, K. R. S. Chandrakumar, S. K. Ghosh;Theor. Chem. Acc.;131(2012) 1205 (1-12).
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2. Unraveling the factors affecting proton transfer energetics of Zundelcation nanoconfined in hydrophobic carbon nanotubes: an ab Initio Study; M. K. Tripathy, N. K. Jena, K. R. S. Chandrakumar, Current Trends in Theoretical Chemistry (CTTC), 1 (2013) 153.

53. Name : **Ram Kumar Singh**
Enrolment No. : LIFE09201004017
Date of Award of degree : 14.06.16
Constituent Institute : Tata Memorial Centre
Title : Molecular imaging of cancer stem cells (CSCs) during development of chemo resistance in ovarian carcinoma.

Abstract

Ovarian cancer is the seventh most common cancer amongst women and ranks 4th in cancer related deaths across the globe. In Indian scenario, it is the 4th most common cancer amongst women. Generation of chemoresistance and relapse are the major hurdle in the disease management. In present thesis we found an enrichment of SP fraction with increased self-renewal and stemness phenotype during acquirement of resistance against cisplatin, paclitaxel and combination treatment in ovarian cancer cells. Real time monitoring of tumor formation with bioluminescence imaging, showed that SP cells from Pac^{ER} stage initiated the tumor formation much earlier than SP cells from Cis^{LR} stage suggesting functional heterogeneity within CSCs. We also reported a preferential regulation of IGF-1R and AKT signaling at early and late resistant stages respectively. While IGF-1R levels were found to be up regulated only at early stages (Cis^{ER}, Pac^{ER} and Cis-Pac^{ER}), higher levels of activated Akt was associated with late resistance. Inhibition of IGF-1R expression resulted in down regulation of stemness like phenotype and stemness gene expression. Thus it is probable that higher IGF-1R expression is required for initiation of resistance development along with maintenance of the CSC like phenotype. Using small molecule inhibitor against IGF-1R auto phosphorylation, we showed increased potentiating cytotoxic effects of chemotherapeutic agents at early stage of resistance. As IGF-1R levels go down in late resistant cells (CisLR, PacLR and Cis-PacLR), it is possible that high level of pAKT maintain the chemoresistance and CSC like phenotype. It would be interesting to identify the transcriptional regulators of IGF-1R and AKT signaling and understand the relation between stemness genes and IGF-1R/Akt signaling at early and late resistant stages in future.

Publications

Journal

1. Ram K Singh, Snehal M. Gaikwad, SmritaChaudhury, Ankit Jinager, AmitaMaheshwari, Pritha Ray, 2014, IGF-1R inhibition potentiates cytotoxic effects of chemotherapeutic agents in early stages of chemoresistant ovarian cancer cells, Cancer Letters, 354 (Aug 22 2014), pp. 254–262

Conferences attended

1. Ram K Singh, Pritha Ray, poster presentation on “Impact of IGF1R/AKT signalling on cancer stem cell heterogeneity and tumorigenicity” at A conference of new ideas in cancer-Challenging dogmas: 26-28 February, 2016, Mumbai, India.
2. Ram K Singh, Ankit Jinager, A. De and Pritha Ray, oral presentation on “IGF-1R: A key linker between chemoresistance and cancer stem cells in epithelial ovarian cancer cells” at “5th Asia Pacific Summit on Cancer Therapy: 20-22 July, 2015, Brisbane, Australia.
3. Ram K Singh, Ankit Jinager, Snehal M. Gaikwad and Pritha Ray “Association of cancer stem/initiating cells with chemoresistance and epithelial-mesenchymal transition in ovarian carcinoma” Poster presentation at XXXVIII All India Cell Biology Conference, 2014 Central Drug Research Institute, Lucknow, India.
4. Ram K Singh, Snehal M Gaikwad, Pritha Ray “The IGF-1R signaling oscillates during acquirement of resistance to cisplatin and paclitaxel in ovarian cancer cells” Poster presentation atXXXVII All India Cell Biology Conference, 2013 in Stem, JN Tata Auditorium, IISC, Bangalore, India.

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6. Ram K Singh and Pritha Ray, "Ovarian Cancer Stem Cells (OCSC) in Acquired Chemoresistance" poster presentation during Asia Oceania research organization on Genital Infections and Neoplasia- India (AOGIN-India), Mumbai, India 2012.

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54. Name : **Satish Kumar Velaga**
Enrolment No. : ENGG02201104020
Date of Award of degree : 14.06.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Comparison Of Weld Characteristics Of Axisymmetrical And Non-Axisymmetrical Butt Welded Pipe Joints.

Publications

Journal

1. A. Ravisankar, Satish Kumar Velaga, Gaurav Rajput, S. Venugopal., Influence of welding speed and power on residual stress during Gas Tungsten Arc Welding (GTAW) of thin sections with constant heat input: A study using numerical simulation and experimental validation. *Journal of Manufacturing Processes*, 2014, Vol. 16, 200-11. http://dx.doi.org/10.1016/j.jmapro.2013.11.002. (ScienceDirect most downloaded article).
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3. Satish K. Velaga, Gaurav Rajput, T. Selvaraj, B.M. Anandarao, A. Ravisankar., A study on the effect of weld induced residual stresses and the influence of weld sequencing of centrifugal extractor rotating bowl using numerical simulation and experimental validation. *Ciência & Tecnologia dos Materiais,* 2015, Vol. 27, 84-91. http://dx.doi.org/10.1016/j.ctmat.2015.03.011 (*journal of the Portuguese Society of Materials).*

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2. Satish K. Velaga, A. Ravisankar, S. Venugopal., Finite element based parametric study on the characterization of GTAW process moving heat source parameters in austenitic stainless steel. Archives of Civil and Mechanical Engineering (ACME).

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2. Satish K. Velaga, Gaurav Rajput, S. Murugan, A. Ravisankar, S. Venugopal., Numerical study on the characterization of Goldak's double ellipsoid heat source parameters in thermal analysis of GTAW process. International congress of International institute of welding - *IC-IIW: 2014,* NewDelhi, India, April 09-11, 2014.
3. Satish K. Velaga, Gaurav Rajput, T. Selvaraj, B.M. Anandarao, A. Ravisankar., A study on the effect of weld induced residual stresses and the influence of weld sequencing of centrifugal extractor rotating bowl using numerical simulation and experimental validation. 2nd International Conference of the International Journal of Structural Integrity - *IJSI: 2014,* Funchal, Madeira, Portugal, September 1-4, 2014.

Publications in National Seminar:

1. Satish K. Velaga, A. Ravisankar, S. Venugopal., Numerical investigation of thermo mechanical behavior during circumferential GTAW process of AISI 304 component. National welding seminar – *NWS: 2015,* Mumbai, India, December 09-11, 2015.
2. Satish K. Velaga, A. Ravisankar, S. Venugopal., Finite element based parametric study of moving heat source model on weld induced residual stress distributions. National welding seminar – *NWS: 2015,* Mumbai, India, December 09-11, 2015.

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55. Name : **Avishek Pal**
Enrolment No. : CHEM01200904023
Date of Award of degree : 14.06.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Development And Characterization Of Charged Membranes For Separation Studies

Abstract

The thesis entitled "*Development and Characterization of Charged Membranes for Separation Studies"* deals with facile development, in-depth studies and extensive investigation as well as performance evaluation of a series of potential charged nanofiltration membranes, which constitute both polymeric as well as polymer – inorganic nanocomposite membranes, all of them being of thin film composite varieties. The membranes developed and studied further include negatively charged as well as positively charged ones derived using innovative chemical formulations leading to filing of two patent applications, two publications in referred journals as well as nine presentations and publications in various conferences. The uniqueness of the studies lies in the fact that the thesis reveals a way of producing membranes containing fixed surface charges in a simple and single step where no post fabrication procedure is required for introduction of charges in to the membranes. The thesis describes the development of negatively charged membranes derived using sulfonic acid containing diamines like 2,4 – diamino benzene sulfonic acid (DABSA) as well as binary sulfonic acid containing monomers such as 4,4/ - diamino stilbene 2,2/ - disulfonic acid (DASDSA) and 2,2/ - benzene disulfonic acid (BDSA). Several membrane compositions have been investigated using binary and ternary recipes, using these monomers, in combination with other amines like piperazine (PIP) and acid chlorides like trimesoyl chloride (TMC) and terephthaloyl chloride (TPC). The thesis describes about positively charged membranes using quaternized polyethyleneimines in shaping the characteristic properties of the membranes. It further deals with an inorganic-polymer nanocomposite membrane derived using nano-ZnO in thin film composite membranes.

Publications

Journal

1. Charged thin film composite nanofiltration membrane and process of its production;Patent Inventors: T. K. Dey, Avishek Pal, R. C. Bindal and P. K. TewariIndian Patent Application No.: 1902 / MUM / 2014, filed on June 10, 2014.
2. Nanofiltration membranes with surface negative charge for fractional separation of mono and multivalent ionic species;Patent Inventors: T. K. Dey, Avishek Pal, R. C. Bindal and P. K. TewariIndian Patent Application No.: 2095 / MUM / 2015, filed on May 29, 2015

Publications in peer-reviewed journals / conference proceedings

1. Nano-ZnO impregnated inorganic–polymer hybrid thin film nanocomposite nanofiltration membranes: an investigation of variation in structure, morphology and transport properties; Avishek Pal, T. K. Dey, Anshu Singhal, R. C. Bindal and P. K. Tewari; RSC Advances, 2015, 5, 34134–34151; DOI: 10.1039/C4RA14854A
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5. Preparation, characterization and performance evaluation of anti-biofouling property of carbon nanotube-polysulfone nanocomposite membranes; Soumitra Kar, M. Subramanian, Avishek Pal, A. K. Ghosh, R. C. Bindal, S. Prabhakar, J. Nuwad, C. G. S. Pillai, S. Chattopadhyay and P. K. Tewari, AIP Conference Proceedings, 2013, 1538 (1),181–185; DOI: 10.1063/1.4810053

Presentations in national / international conferences:

i. Effect of compositional variations of amine component, containing 2, 4 - diamino benzene sulfonic acid and piperazine, on the performance of negatively charged thin film composite nanofiltration membranes, Avishek Pal, T. K. Dey, R. C. Bindal, S. Prabhakar and P. K. Tewari, SIII-3; Oral Presentation, National conference on water purification technologies and management (InDACON) – 2012, Navi Mumbai, India.

ii. Study of separation characteristics of indigenously developed negatively charged nanofiltration membranes towards single and binary mixed electrolyte systems; Avishek Pal, T. K. Dey, R. C. Bindal, S. Prabhakar and P. K. Tewari, pp. SIII-12; Poster Presentation, National conference on water purification technologies and management (InDACON) – 2012, Navi Mumbai, India.

iii. Effect of acid chlorides as reactant on the morphology and performance of negatively charged thin film composite nanofiltration membranes; Avishek Pal, T. K. Dey, R. C. Bindal, S. Prabhakar and P. K. Tewari, pp. 52; Poster Presentation, DAE-BRNS symposium on emerging trends in separation science and technology (SESTEC) – 2012, Mumbai, India.

iv. Impact of curing conditions on surface features of thin film composite nanofiltration membranes: An AFM - SEM study; Avishek Pal, T. K. Dey, R. C. Bindal and P. K. Tewari, pp. 74; Oral Presentation, Third international multicomponent polymer conference (IMPC) – 2012, Kerala, India.

v. Influence of electrolytes on the electro-kinetic behaviours of charged nanofiltration membrane; Avishek Pal, T. K. Dey, R. C. Bindal and P. K. Tewari, pp. 43; Oral Presentation, International conference on water desalination, treatment and management (InDACON) – 2013, Jaipur, India.

vi. Synthesis, characterization and antibiofouling performance evaluation of graphene and graphene oxide embedded polysulfone nanocomposite ultrafiltration membranes; Soumitra Kar, Avishek Pal, Mahesh Subramanium, Nitesh Goshwami, R. C. Bindal, S. Chattopadhyay and P. K. Tewari, pp. 73; Oral Presentation, International conference on water desalination, treatment and management (InDACON) – 2013, Jaipur, India.

vii. Preparation and physicochemical characterization of a crosslinked & quaternized polyamide network based positively charged thin film composite nanofiltration membrane; Avishek Pal, T. K. Dey, R. C. Bindal and P. K. Tewari, pp. 223; Poster Presentation, DAE-BRNS symposium on emerging trends in separation science and technology (SESTEC) – 2014, Mumbai, India.

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ix. Analysis of amplitude parameter-linked surface topographies of nanofiltration membranes using atomic force microscopy; Avishek Pal, T. K. Dey, R. C. Bindal and P. K. Tewari, pp. 353-361; Oral Presentation, International conference on innovative technologies and management for water security (InDACON) – 2014, Chennai, India.

x. Dependence of performance of positively charged nanofiltration membranes on molecular weight of poly(ethyleneimine), Avishek Pal, T. K. Dey, R. C. Bindal and P. K. Tewari, pp. 265-269; Poster Presentation, Trombay symposium on desalination and water reuse (TSDWR) – 2015, Mumbai, India.

56. Name : **Sandipan De**
Enrolment No. : MATH10201004007
Date of Award of degree : 21.06.16
Constituent Institute : Institute of Mathematical Sciences,
Title : Infinite Iterated Crossed Products Of Hopf Algebras, Drinfeld Doubles And Planar Algebras

Abstract

This thesis deals with the mathematical objects known as planar algebrasand their connection with Hopf algebras and their Drinfeld doubles.The motivation for this thesis comes from a folklore result in subfactor theory which asserts that for a Kac algebra subfactor, a related subfactor to its asymptotic inclusion comes from an outer action of its Drinfeld double. In the process of trying to prove this, we obtain a purely algebraic result which is one of the main results in the thesis. The result is roughly the following. Given finite-dimensional Hopf algebra over any field, we associate to it a very natural inclusion A in B of infinite iterated crossed product algebras and show that B is the crossed product of A by the Drinfeld double of the given Hopf algebra. More significantly, we show that Drinfeld double is the only finite-dimensional Hopf algebra with this property and thus produce a context in which the Drinfeld double arises very naturally. Further, we produce an explicit embedding of the planar algebra of the Drinfeld double of a finite-dimensional semisimple, cosemisimple Hopf al- gebra over an algebraically closed field into the two-cabling of the planar algebra of the dual Hopf algebra and give a characterisation of the image.

Publications

Journal

1. \Note on infinite iterated crossed products of Hopf algebras and the Drinfeld double", Sandipan De and Vijay Kodiyalam, Journal of Pure and Applied Algebra, 2015, 219 Vol. 12, 5305 - 5313.

Preprints

1. Planar algebras, cabling and the Drinfeld double", Sandipan De andVijay Kodiyalam, (2016).

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57. Name : **B. Krishna Srihari**
Enrolment No. : ENGG02201104011
Date of Award of degree : 21.06.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Modeling the electrorefining process and the effect of cathode design in a molten salt electrorefiner.

Abstract

The fuel discharged from a nuclear reactor after irradiation still contains most of the fertile material (U^{238} or Th^{232}) which was also the major constituent of the virgin fuel, significant amounts valuable fissile nuclides

(U^{235}, U^{239} and/or U^{233}) and large amounts of fission products. Reprocessing of the spent fuel is aimed at (1) recovering uranium and plutonium and thorium if present, for reuse as nuclear fuels and (2) removing the fission products. Pyrochemical reprocessing is one of the non-aqueous processes and among them; molten salt electrorefining is a pyrochemical reprocessing method especially advantageous for treating metallic fuels from FBR's.The following modeling and experimental work on the design of electrodes for the electrorefiner were carried out in this study and these will be discussed in the thesis: Developed the model for the electrorefining process using COMSOL Multiphysics in which three modules of the software were coupled together and studied the electrotransport behavior of uranium and plutonium from liquid cadmium anode to solid cathode and validated the model with experimental data from literature.Developed the model to study the effect of the electrode configuration for achieving higher throughput and validated the model with experimental studies carried out by us as well as with experimental data from literature. Also studied the electrodeposition of uranium using different shapes of the cathode both by modeling and by experimental work. Simulated the concentration variation of U and Pu and Pu/U ratio's in the molten salt, liquid cadmium anode and amount of U deposit on the solid cathode and validated with literature data. Also predicted the cell voltage and compared with literature data. Evaluated the potential and current density distributions, measured the current and calculated the cell resistance. Compared the cell resistance of present model with present experimental results and also with literature. Electrodepositions of uranium on three different shapes of cathode were performed. As a first approach, taken equal surface areas and in the second approach maintained equal immersion height. The validated results of present model are good agreement with the experimental results.

Publications

Journal

1. B. Krishna Srihari, S. Agarwal, B. Prabhakara Reddy, P. M. Satya Sai, B. Muralidharan & K. Nagarajan (2015) "Modeling The Molten Salt Electrorefining Process For Spent Metal Fuel Using COMSOL", Separation Science And Technology, 50:15, 2276-2283.
2. B. Krishna Srihari, B. Prabhakara Reddy, P. Venkatesh, S. Agarwal, P. M. Satya Sai & K. Nagarajan (2016) "Experimental Studies And Model Validation For The Optimization Of Electrode Configuration In A Molten Salt Electrorefiner", Separation Science And Technology, DOI: 10.1080/01496395.2016.1158190.

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1. Bonasi Krishna Srihari, B. Prabhakara Reddy, P Venkatesh, K. Nagarajan, "Optimizing electrode surface area by Comsol Multiphysics", presented poster during COMSOL Conference -2013, Bengaluru, October 17-18, 2013.
2. Bonasi Krishna Srihari, Sourabh Agarwal, B. Prabhakara Reddy, K. Nagarajan, "Effect of electrode configuration on the current and potential distribution in a molten salt electrorefiner", presented poster during International Conference on Electrochemical Science and Technology -2014, IISc Bengaluru, August 7-9, 2014.

58. Name : **Deepak Tyagi**
Enrolment No. : CHEM01201004010
Date of Award of degree : 21.06.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Development of Catalysts for Hydriodic Acid Decomposition Reaction for Hydrogen Generation from Thermochemical Cycles

Abstract

Hydrogen is an attractive energy carrier for future energy demands if it can be produced from water in an economical and environment friendly way. One of the methods for large scale production from water is thermochemical cycles. Sulfur-Iodine thermochemical cycle is proposed for the large scale production of hydrogen employing nuclear or solar heat. This thesis reports development of catalysts for hydriodic acid decomposition reaction; the hydrogen producing step of S-I thermochemical cycle as well as other iodine based cycles.Majority of work and catalytic systems for HI decomposition reported in open literature are for vapor phase decomposition, while in this work detailed evaluation has been carried out for various catalysts under liquid phase decomposition of HI.Platinum based catalysts with carbon supports as well oxide supports have been explored for the reaction. In case of carbon supports, catalysts with varying properties like surface area and pore structure has been prepared by different methods like wet impregnation method, hard templating method etc. These catalysts have been extensively characterized for their structure and morphology. These catalysts are also evaluated for their activity for liquid phase HI decomposition reaction.Catalyst stability has also been studied by examining the used catalyst and by determining the extent of platinum leaching under reaction conditions.Effect of noble metal loading has also been delineated for Pt/carbon catalysts. From these studies, it was found that the support with mesoporous and planar type of structure are more active as compared to microporous catalysts. Platinum based catalysts supported on oxides like zirconia, ceria and titania have also been studied. These catalysts have been characterized by using various techniques for their structure and morphology and studied for their activity for liquid phase HI decomposition reaction.Zirconia supported catalysts was found to be performing better as compared to the other two oxide catalysts in terms of activity and stability. In connection to iodine speciation studies, UV visible absorption spectroscopy and Raman spectroscopy studies were used confirm the presence of I_3^- and higher polyiodides in the HI_x phase of Bunsen reaction of sulfur Iodine thermochemical cycle.

Publications

Journal

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2. Iodine speciation studies on Bunsen reaction of S-I cycle using spectroscopic techniques;Deepak Tyagi, Salil Varma, K. Bhattacharya, D. Jain, A. K. Tripathi, C. G. S. Pillai and S. R. Bharadwaj, *International Journal of Hydrogen Energy*, 37 (2012) 3621-3625.
3. Pt/zirconia catalyst for hydrogen generation from HI decomposition reaction of S-I cycle; Deepak Tyagi, Salil Varma and S. R. Bharadwaj, *International Journal of Energy Research*, 39(2015) 484-493.
4. Pt/graphite catalyst for HI decomposition reaction in sulfur - iodine thermo-chemical cycle; Deepak Tyagi, Salil Varma and S. R. Bharadwaj, *International Journal of Energy Research,* 39(2015) 2008-2018.
5. Mesoporous carbon supported platinum nano-catalyst: Application for Hydrogen production by HI decomposition reaction in S-I cycle; Deepak Tyagi, S. Varma and S. R. Bharadwaj, *Journal of Nanoscience and Nanotechnology,* (doi:10.1166/jnn.2016.12812)

6. Pt catalysts supported on carbon derived from rice: Application for HI decomposition reaction of S-I cycle; Deepak Tyagi, Salil Varma and S. R. Bharadwaj, *International Journal of Green Energy* (Submitted)
7. Comparative activity and stability of oxide supported platinum catalysts for HI decomposition reaction of S-I cycle; Deepak Tyagi, Salil Varma and S. R. Bharadwaj, *International Journal of Energy Research* (To be submitted)
   37-44.

Conference:

1. Development of Pt- Carbon Catalysts for HI Decomposition Reaction in S-I thermochemical Cycle Using Hard Templating Route ; D. Tyagi, K. Scholz, S. Varma, K. Bhattacharyya, and S.R. Bharadwaj; Proc. of 3rd International Symposium on Materials Chemistry, BARC, Mumbai December 2010. Page- 317.
2. Iodine speciation studies on Bunsen Reaction of S-I cycle using Spectroscopic techniques; Deepak Tyagi, Salil Varma, K. Bhattacharya, D. Jain, A. K. Tripathi, C. G. S. Pillai and S. R. Bharadwaj; International conference on Renewable Energy (ICRE-2011) , Jaipur, Jan 2011
3. Development of Pt-Carbon Catalysts using MCM-41 template for HI decomposition reaction in S-I Thermochemical Cycle; Deepak Tyagi, K. Scholz, S. Varma, K. Bhattacharya, S. Mali, P. S. Patil and S. R. Bharadwaj; International conference on Renewable Energy (ICRE-2011) , Jaipur, Jan 2011
4. Pt-Carbon catalysts by hard templating route; Deepak Tyagi, Salil Varma, A. N. Shirsat and S. R. Bharadwaj; Proceedings of the 18th International Symposium on Thermal Analysis (THERMANS-2012). Page 239-245
5. Pt/Graphite catalyst for HI decomposition reaction in Sulphur - Iodine thermochemical Cycle; Deepak Tyagi, Salil Varma, S. R. Bharadwaj, Proceedings of National conference on Carbon Materials 2012 (CCM12), Page 64.
6. Mesoporous Pt/carbon catalyst by Hard Templating Route using SBA-15 as a Template; Deepak Tyagi, Salil Varma, W.-D. Einicke, S. R. Bharadwaj and R. Gläser; Proceedings of National conference on Carbon Materials 2012 (CCM12), Page 159.
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8. Pt/Titania catalyst for liquid phase HI decomposition reaction of Sulphur - Iodine Thermochemical Cycle, Deepak Tyagi, Salil Varma, Shyamala R. Bharadwaj Paper presented at 21st National Symposium on Catalysis “Catalysis for Sustainable Development” (CATSYMP-21) at IICT, Hyderabad during 10 to 13 Feb 2013, Page-75
9. Development of Pt/Zirconia catalyst for liquid phase HI decomposition reaction in S-I cycle Deepak Tyagi, Alisha Gogia, Salil Varma, A. K. Tripathi, S. R. Bharadwaj, Proc.4th Int. Conf. on Advances in Energy Research, IIT, Bombay, Dec. 10 -12, 2013, page 57.
10. Role of Carbon support on Activity and Stability of Pt/C catalyst for Hydrogen production by S-I thermochemical cycle; D. Tyagi, S. Varma, S. R. Bharadwaj, Materials Challenges in Alternative and Renewable Energy (MCARE-2014) February 17-20, 2014 | Hilton Clearwater Beach Resort, Clearwater, Florida, USA
11. Development of Novel Catalytic systems for reactions involved in Hydrogen generation from Thermochemical Cycles presented at 26th Research Scholars' Meet 2014 (RSM-2014)organized by Indian Chemical Society at C.K.T, College, Panvel during February 21-22,2014.
12. A Comparative Study of Pt catalysts supported on different oxide supports for HI decomposition: The Hydrogen producing step in S-I Thermochemical Cycle Proc. of 5th Interdisciplinary Symposium on Materials Chemistry (ISMC 2014), BARC, Mumbai December 2014.

13. Pt/Carbon catalyst for Hydrogen production by S-I thermochemical cycle: Effect of Pore structure of Carbon support; Deepak Tyagi, Salil Varma, S. R. Bharadwaj; 22st National Symposium on Catalysis “Catalysis for Better Tomorrow” (CATSYMP-22) at CSIR-CSMCRI , Bhavnagar during 07 to 09 Jan 2015, Page-125-126.

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59. Name : **P. Dhanasekaran**
Enrolment No. : ENGG02200904010
Date of Award of degree : 21.06.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Arsenic And Fluoride Removal From Drinking Water By A Novel Adsorbent

Abstract

Arsenic contaminated drinking water has been found in India (West Bengal), Bangladesh, Southeast Asian deltas. Arsenic and fluoride present together above WHO levels in Pakistan, Tanzania, and India. As per the BIS, a maximum acceptable limit for arsenic is 0.01 mg/L and fluoride 1 mg/L for drinking water. Arsenic is classified as a Group I carcinogen (human carcinogen). Fluorosis caused by intake of high fluoride containing water. A novel adsorbent was synthesized by impregnating the Anjili tree sawdust with Ferric hydroxide and Activated Alumina (SFAA) in the mass ratio of 1.5:1:1 was chosen based on its high adsorption capacity of As, F. This adsorbent is economic, ecofriendly and minimizes generation of secondary wastes. The treated water conforms to WHO limits for potable water, with respect to arsenic, fluoride, iron and aluminium.ICP-MS and ion selective electrode have been used for arsenic and fluoride analysis. BET surface area, pore volume and pore size distribution of sawdust, SFAA, As(V), As(III) and fluoride adsorbed SFAA were identified by liquid N_2 adsorption method and Mercury porosimetry. The SEM-EDX studies shows the presence of Al, Fe, As(V), As(III), F in SFAA after adsorption. FTIR study confirms that SFAA contains several functional groups on its surface of SFAA. The XPS survey gave the signatures of As 3d, As 3p, F 1s, C 1s, O 1s and Fe 2p. Point of Zero Charge of SFAA was 5.85. Arsenic adsorbed in the pH range of 6.5-7.0. Upto pH 9 the fluoride adsorption was constant and beyond 9 it decreased. The maximum equilibrium uptake capacities were found to be 77.60 mg/g, 54.32 mg/g and 40.28 mg/g for As(V), As(III) and fluoride respectively. As(V) adsorption, both electrostatic attraction and chemical bonding take place. But in case of As(III), only chemisorption takes place. As(V), As(III), fluoride and As+F adsorption by SFAA follows Freundlich isotherm and pseudo second order kinetic model. Thermodynamic studies gave three basic thermodynamic parameters for arsenic and fluoride are, standard enthalpy (ΔH^o = 13.57 & 17.86 KJ/mol), standard entropy (ΔS^o = 0.138 & 0.1 KJ/mol.K) and standard free energy (ΔG^o). The value of ΔH^o indicates that the process is chemisorption, negative value of ΔG^o indicates the process is spontaneous. Interference of other ions on As(V) adsorption by SFAA was observed to be in the order of $PO_4^{3-} > SO_4^- > HCO_3^- > NO_3^-$. For fluoride adsorption the order be $OH^- > CO_3^{2-} > HCO_3^- > NO_3^- > SO_4^{2-} > Cl^-$. Fixed bed adsorption by SFAA was higher than that of activated alumina. Fixed bed adsorption of As(V), fluoride and As(V)+F using SFAA by varying the flow rate, particle size, initial concentration and bed height were studied and optimum operating parameters were established. Column experiments showed that removal of As(V), fluoride and As(V)+F from water was better for low flow rates, small particle sizes, low initial concentrations and large adsorbent bed heights. Thomas, Yoon-Nelson, Bohart-Adam and Clark models were tested with the experimental data and model parameters were estimated. Clark model explained arsenic, fluoride and As(V)+F adsorption by SFAA well.

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2. Defluoridation of water by chemical impregnated *Artocarpus hirsutus* sawdust, Water Science and Technology: Water supply, DOI: 10.2166/ws.2016.032
3. Fixed bed adsorption of arsenic from water by chemical impregnated *Artocarpus hirsutus* sawdust, Journal of Environmental Sciences (Under Review)
4. Fixed bed adsorption of fluoride by *Artocarpus hirsutus* based adsorbent, Journal of Fluorine Chemistry (Communicated)
5. Arsenic and fluoride adsorption from water by Aanjili tree sawdust impregnated with ferric hydroxide and activated alumina, Separation Science and Technology (Under Review)

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3. Arsenic removal from drinking water by a novel adsorbent, International Conference on Innovative Technologies and Management for Water Security, INDACON-2014, NIOT, Chennai, India, 12-14 February 2014.
4. Arsenic(V) removal from drinking water by modified adsorbent, SESTEC-2012, Bhabha Atomic Research Centre, Mumbai, India. February 27 – March 1, 2012.

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60. Name : **Makkuva Kalyan Phani**
Enrolment No. : ENGG02201004018
Date of Award of degree : 21.06.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Quantitative Mapping Of Elastic Properties In Nickel And Titanium Base Alloys At Nanoscale Using Atomic Force Acoustic Microscopy.

Abstract

Atomic force acoustic microscopy (AFAM) was used for mapping the elastic modulus of various phases/precipitates present in two main classes of multiphase structural alloys viz. nickel and titanium alloys, at nanoscale. The microstructure of the multiphase alloys were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), electron back scatter diffraction (EBSD) and Atomic force microscopy (AFM) studies. Specific software were developed to acquire and analyze the data obtained by AFAM systemIn nickel base superalloys, a polycrystalline superalloy,alloy 625 and a directionally solidifiedsuperalloy,CM 247A were taken for study. A new methodology was developed to circumvent the problem of change in tip radius by implementing simultaneous acquisition of two contact resonance frequencies and by using matrix as a reference. Cantilever dynamics model neglecting damping was used to derive the contact stiffness (k^*) and indentation modulus (*M*). Experimental M values of γ', δ and carbides present in the two nickel base superalloys were reported for the first time. Simultaneous mapping of stiffness and damping was carried out in two types of titanium base alloys. Ti-6Al-4V, an$\alpha+\beta$ titanium alloy and Ti-10V-4.5Fe-1.5Al, aβ titanium alloy were taken for

study. Specimens of titanium alloys were subjected to heat treatment at different temperatures. Cantilever dynamics model considering damping was used to derive the M and damping (E''/E'). The experimental M and E''/E' values of α, β and α'phases present in the two titanium alloys were reported for the first time.Effect of heat treatment temperature and duration on the elastic and damping properties was studied. The elastic and damping properties at nanoscale are compared with those for bulk samples by ultrasonic measurements. The study demonstrated that the nanoscale elastic properties measured using AFAM can also be used for obtaining the average elastic properties of the bulk samples with an accuracy of ~5 %. The systematic error in the elastic property measurements using single reference has also been brought out. Attempts were made to understand the effect of crystallographic orientation on AFAM measurements. It was demonstrated that, due to the close packed orientation relationships of precipitates with the matrix, the modulus of a precipitate measured by the methodology described in the present thesis was not affected to a large extent by the orientation of individual grain in which the measurement was made. The study also clearly demonstrates that, AFAM can be used to disclose relative elastic property of materials with high spatial resolutions,even for materials with a slight difference in elastic properties (~4 %).

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2. M. Kalyan Phani and Anish Kumar, “Elasticity mapping of precipitates present in CM247A aeronautical grade superalloy using atomic force acoustic microscopy”, presented at 2nd International Conference on Advances in Steel, Power and Construction Technology” held at OP Jindal University, Raigarh, India, March2016.
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1. M. Kalyan Phani, Anish Kumar and T. Jayakumar,“Elasticity mapping of sub-micron size precipitates in Inconel 625 using Atomic Force Acoustic Microscopy” presented at 50th National Metallurgists Day – Annual Technical Meet(NMD-ATM)held at Jamshedpur, India, November 2012.
2. Anish Kumar, M Kalyan Phani, S. Sosamma, B.P.C. Rao and T. Jayakumar, “Multi-scale microstructural characterization through acoustic measurements”, presented at Acoustics held at New Delhi, India, November 2013.

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61.	Name	:	**Abhik Mukherjee**
	Enrolment No.	:	PHYS05201004003
	Date of Award of degree	:	21.06.16
	Constituent Institute	:	Saha Institute of Nuclear Physics,
	Title	:	Study Of Nonlinear Waves In Oceanic And Other Physical Systems

Abstract

Near shore surging waves like tsunami, bore waves etc have hazardous nature when it propagates towards the shore. We have proposed in this thesis work, a direct method to control the near shore surging waves, which could reduce the hazardous effects. A leakage based method is proposed here, which would suck water at the bottom causing the properties of solitary waves to change. It has been shown analytically that if the vertical fluid velocity at the bottom is independent of the free surface wave profile then the phase of the solitary wave gets changed controlled by the bottom boundary condition, whereas the amplitude remaining constant. But if the leakage function depends on the surface wave profile then a variable KdV equation can be derived for slowly changing bathymetry function. An exact solitary wave solution is obtained for a finer balance between the variable depth function and leakage function .The amplitude of the solution decreases as it propagates towards the shore in spite of the surging nature due to decreasing bathymetry. In the second part of the thesis the deep water rogue wave phenomena has been modelled. In this context, a new completely integrable, (2+1) dimensional, local, modulated, nonlinear, evolution, equation has been proposed which is derivable from the basic hydrodynamic equations. The most important part is that this equation possesses an exact two dimensional rational solution which is analogous with the Peregrine breather in terms of mathematical form. Also it contains two free parameters which can be chosen arbitrarily to model the full grown rogue wave. As an extension to the problem, we have also derived this new, (2+1)D, evolution equation in the propagation of nonlinear ion acoustic wave of lossless, magnetized plasma. As an applications to these integrable models, which have been discussed, we explored different physical systems like inhomogeneous plasma, quantum plasma and derived various interesting results.

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62. Name : **Harishchandra Singh**
Enrolment No. : PHYS03201004011
Date of Award of degree : 23.06.16
Constituent Institute : Raja Ramanna Centre for Advanced Technology,
Title : Structural and Spectroscopic studies of transition metal based Multiferroics and Oxides.

Abstract

The thesis reports investigation of structural and spectroscopic properties of transition metal based magneto-electric multiferroic systems and their correlation with the magnetic as well as ferroelectric properties. Low structural symmetry systems Co3TeO6 (CTO) and Mn doped CTO (CMTO) have been synthesised using an optimized solid state reaction route and their growth mechanism has been studied. Further, Cobalt is found to exist in mixed oxidation states of +2 and +3, which gives rise to the possibilities of both ferromagnetic (FM) and antiferromagnetic (AFM) interactions, in CTO. With the help of low magnetic field magnetization, it is established that CTO show short range FM interactions in addition to reported AFM interactions, the so called Griffiths Phase (GP). We have observed five AFM transitions, which are understood to be due to four Co-O-Co networks corresponding to five crystallographically in-equivalent lattice sites of Co. Experimental observations of spontaneous polarization as well as spontaneous magnetization and magneto-dielectric coupling (representing spin lattice coupling in this system) have been reported in CTO, for the first time. Further, Mn doping in CTO increases the critical temperature (below which the samples attain AFM interactions) substantially. In this work, the reason for the increase in AFM transition temperature is attributed to decreased TM-O bond lengths as well as maximum average TM charge states for a specific concentration of Mn. The observance of robust FM interactions (below 185 K) in CMTO systems shows supersession on increasing the magnetic fields. The FM transitions are limited to short range length scales and are embedded in long range AFM matrix (GP similar to the case of CTO). GP is found to be much more robust (compared to CTO), in the sense that it shows up to much higher magnetic fields and higher temperatures. The thesis is organized in five chapters. The Introduction chapter describes the importance and status (before this thesis) of the present work. In chapter 2, synthesis method and characterization techniques have been described. An important contribution of this chapter is establishment of X-ray absorption near edge structure (XANES) spectroscopy technique for study of phase concentration of Co3O4 and CoO in a mixed phase samples. Chapter 3 and 4 covers the main results of the thesis along with discussion on results. In the final chapter, conclusion of this work and scope for future work has been listed

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8. Insight into the growth reaction mechanism of ceramic Co3TeO6: Synchrotron structural and thermal analysis; Harishchandra Singh, A. K. Sinha, S. M. Gupta, M. N. Singh, H. Ghosh; Journal of the American Ceramic Society: in press

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63. Name : **K. Anand Rao**
Enrolment No. : ENGG01200904032
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Constituent Institute : Bhabha Atomic Research Centre,
Title : Carbonate Leaching Of Uranium From Indian Alkaline Host Rocks Using Oxygen: Mathematical Modeling And Experimental Validation

Abstract

The thesis provides a detailed account of the mathematical modeling and experimental validation of the kinetics of carbonate leaching of uranium, using oxygen, from two prominent deposits of alkaline host rocks in India namely, Tummalapalle in Andhra Pradesh and Gogi in Karnataka. The former is a lean tenor (0.03 –

0.04% U_3O_8) deposit that has potential to become one of the large deposits in the world. The latter is of medium (0.15 – 0.2% U_3O_8), but highest, grade deposit discovered in India so far.Exhaustive characterization studies carried out on the feed materials used in leaching experiments included optical microscopy, X-ray diffractometry, BET surface area measurements, wet chemical analysis by Fluorimeter and UV/Visible spectrophotometer. The advanced instruments like Scanning Electron Microscope and Inductively Coupled Plasma-Optical Emission Spectrometer (ICP-OES) have also been used to characterize the samples investigated for carbonate leaching of uranium. The leaching rate models were developed for single and binary synthetic mixtures of pure uranium dioxide and pyrite mineral. Michaelis Menton type of model equation was developed for dissolution of pure UO_2. Leaching of pure pyrite followed chemical reaction controlled shrinking core model. The presence of pyrite up to 3% (by wt) was beneficial for uranium leaching, but beyond 3 wt%, it was detrimental to carbonate leaching of synthetic mixture of minerals at $T = 398$ K and $p_{O2} = 5.2$ atm. The basic studies carried out on synthetic mixtures were followed by modeling of the kinetics of batch leaching of ore samples from Indian alkaline host rocks both in the absence and presence of oxygen gas. Pore diffusion controlled model incorporating particle size distribution was found to be most applicable for leaching of uranium from Tummalapalle ore. Topochemical reaction controlled model coupled with particle size distribution best represents the leaching of uranium from Gogi uranium ore. The leaching models of pure UO_2 cannot be directly used for uranium ores. Oxygen is essential for dissolution of uranium. However, specific ores may show some dissolution of uranium values even in the absence of oxygen because of the possible UO_3 content of uranium minerals present in the ore. Leaching results were corroborated with in-depth optical and scanning electron microscopic images showing the morphological changes that occur during leaching of the pure minerals, uraninite and pyrite, vis-a-vis two Indian uranium ores.The batch leaching kinetics (obtained in a 5 L capacity autoclave) of Tummalapalle uranium ore has been scaled to multiple continuous stirred reactors using an improved Residence Time Distribution (RTD) model.The predicted temperatures of pulp at different residence times matched well with measurements on a pilot scale continuous reactor (volume = 850 L). The residence time scale model could even predict the leaching efficiencies of uranium and pyrite values, and temperature of the contents in a commercial reactor, about 800 times the size of pilot scale reactor. The predictions are useful not only to design continuous leaching of uranium ore on a commercial scale but also to find the limit on pyrite content of the ore to operate commercial reactors below design temperature.

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2. Application of a topochemical reaction model to predict leaching behavior of high carbonate uranium ores in alkaline solutions: An experimental case study. K.Anand Rao and A.K.Suri, *Hydrometallurgy*, 141 (2014) 67–75. (http://dx.doi.org/10.1016/j.hydromet.2013.10.005).
3. Kinetics of alkaline leaching of UO_2 and FeS_2 in co-existing system. K. Anand Rao, T. Sreenivas, MadhuVinjamur, A.K. Suri, *Transactions of the Indian Institute of Metals*, 69(1) (2016) 23-31. (http://dx.doi.org/10.1007/s12666-015-0615-8).

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2. Leaching kinetics of UO_2 and FeS_2 in co-existing systems under oxidative alkaline conditions.K. Anand Rao, T. Sreenivas and MadhuVinjamur, Proceedings of 52nd National Metallurgists Day and 68th Annual Technical Meeting of the Indian Institute of Metals (NMD-ATM-2014) held at Pune, India during 12-15 Nov’2014.
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6. Process development studies for low-grade uranium deposit in alkaline host rocks of Tummalapalle. A.K. Suri, N.P.H Padmanabhan, T.Sreenivas, K. Anand Rao, A.K. Singh, K.T.Shenoy, T. Mishra and S.K. Ghosh. Proceedings of IAEA Technical Meeting on Low-grade uranium deposits at Vienna, March 2010.

64. Name : **Sandeep Rimza**
Enrolment No. : ENGG06201104004
Date of Award of degree : 13.07.16
Constituent Institute : Institute For Plasma Research
Title : Studies On Helium Cooled Plasma Facing Components For Tokamak Based Fusion Reactor Applications.

Abstract

It is generally accepted that fusion power is one of the promising sources of sustainable energy in the future. Towards development of fusion reactor technology, India is seriously pursuing research and development activities through Department of Atomic Energy (DAE) at the Institute for Plasma Research along with support from other DAE as well as Non-DAE institutions. The study was launched with the aim of developing an innovative power plant concept for future fusion reactor known as “DEMO” reactor. However, there are many challenges towards successful design of the DEMO. One among them is the design of the divertor which is an important part of the fusion reactor that handles extremely high heat and particle flux escaping from the hot core plasma region along Scrape-Off-Layer (SOL). The function of the divertor is to remove fusion ash, plasma impurities, and unburned fuel from the reactor which affects the quality of the plasma. The entire divertor system is typically divided into a number of modules known as “Cassettes” for improved handling, assembly/dis-assembly, repair and maintenance. Each cassette consists of plasma facing “Divertor targets” with respective support structures and coolant supply network. Each divertor target is made of tungsten material with appropriate cooling mechanism to extract the heat energy. Tungsten (W) is the preferred choice to be used as plasma facing material for covering the entire surface of divertor target due to its excellent thermo-physical properties such as high melting point, low thermal expansion, high thermal conductivity, low tritium retention, low erosion/sputtering rate, low-neutronic activation. In the present helium cooled divertor concept study, divertor target is made up of numerous “finger” type assemblies cooled using high pressure high temperature helium gas to extract the heat energy. Helium gas has been chosen as the coolant due to its favourable safety characteristics and its ability to operate at high temperatures, which enhances the thermal efficiency of the power conversion systems. However, major drawbacks are its comparatively poor heat exchange capability and considerably large pumping power requirement. In the context of DEMO, it is desirable to explore efficient cooling technology for helium cooled divertor, which can withstand high heat flux values of ~10 MW/m2.

Towards this, a novel design for heat transfer enhancement of helium cooled divertor finger mock-up has been proposed. Heat transfer characteristics of finger mock-up have been numerically investigated with new sectorial extended surfaces (SES). Numerical investigations show that addition of SES greatly increases thermal-hydraulic performance of the finger mock-up. Detailed parametric studies on critical parameters that influence thermal performance of the finger mock-up have been analysed. Thermo-mechanical analysis has also been carried out through finite element based approach to know the state of stress in the assembly as a result of large temperature gradients. It is seen that the stresses are within the permissible limits for the divertor design. In order to validate the findings, experimental and computational approach has been proposed for the evaluation of thermal hydraulics performance of a finger type divertor with SES. Critical thermal hydraulic parameters, effective heat transfer coefficient and pressure loss have been measured in the experiment for the reference divertor as well as for a divertor with SES. The thermal performance has been evaluated by comparing the heat transfer coefficient and pressure drop across the test section. The experimental mock-ups are made to full scale respecting Reynolds and Prandtl number similarities. Air is used as the simulant to represent helium, which is the coolant in prototype. Heat concentrator has been developed to simulate high heat flux, by electrical heating. The benchmark experimental data have been used to validate the three dimensional conjugate heat transfer models. The computational result for heat transfer coefficients and pressure loss are in satisfactory agreement with the experimental results. Based on detailed parametric studies, correlations have been proposed for Nusselt number (Nu) and pressure loss coefficient (KL) as a function of Reynolds number which can be used for design applications. The proposed

SES divertor is seen to significantly augment the thermal performance of the finger type divertor at the penalty of a minimum pressure drop at the prototypical condition. The results of the present study provide added confidence in the numerical model used to design the divertor and its applicability to other high heat flux gas cooled components. Following satisfactory validation, elaborate parametric studies have been carried out towards geometrical optimization of divertor finger mock-up with SES to enhance the thermal hydraulic performance. Various non dimensional design variables, viz., relative pitch, thickness, jet diameter, the ratio of height of SES to jet diameter and circumferential position of the SES are considered for the optimization study. The analysis reveals that, the heat transfer performance of finger mock-up with SES is improved for two optimum designs having relative pitch and thickness of 0.30 and 0.56 respectively. Also, it is observed that finger mock-up heat sink with SES performs better, when the ratio of SES height to jet diameter, reduces to 0.75 at the cost of marginally higher pumping power. The effects of jet diameter and circumferential position of SES are found to be counterproductive towards the heat transfer performance. To understand the stress distribution in the optimized geometries, a combined computational fluid dynamics and structural analysis has been carried out. It is found that deviation in peak stresses among various optimized geometries is not significant. Development of an efficient divertor concept is an important task to meet in the scenario of the fusion power plant. Therefore, an innovative divertor heat sink concept cooled by helium is proposed for the fusion reactor. The first wall of the divertor made-up of several modules has to overcome the stresses caused by high heat flux, in the proposed design. Thermal hydraulic performance of one such divertor heat sink module is numerically investigated. The effects of critical thermal hydraulic and geometric parameters on the heat transfer characteristics are investigated as a function of Reynolds number. The 3-dimensional thermal hydraulic investigations include thimble diameter (DT), nozzle diameter (DN), the ratio of nozzle to wall space and nozzle diameter (H/DN) and nozzle shapes etc. as parameters. Elliptical nozzles at specific orientation are found to perform better than other nozzles for identical Reynolds number. The performances of triangular nozzles are found to be poorer than other nozzles. Similarly, a minimum thimble temperature and pressure drop in the circuit is achieved at H/DN ~1.66. The proposed design is found to have a margin of 10 % i.e., capable of handling 11 MW/m2 against target heat flux values of 10 MW/m2.The stresses induced in the divertor heat sink by the thermal and pressure loads are important factors that limit the life of the divertor. Therefore, structural analysis of the divertor heat sink assembly has been carried out and the stress values arising out of temperature gradient and pressure are found to be within acceptable limits, demanding the reliability of the proposed concept.

Publications

Journal

Accepted:

1. "Computational fluid dynamic studies on plasma facing heat sink concept for tokamak application", **S. Rimza**, S. Khirwadkar, K. Velusamy, *Applied Thermal Engineering (Elsevier),* **2016**, 100, 1274–1291.
2. "Optimal design of divertor heat sink with different geometric configurations of sectorial extended surfaces", **S. Rimza**, K. Satpathy, S. Khirwadkar, K. Velusamy, *Fusion Engineering and Design (Elsevier),* **2015**, 100, 581–595.
3. "An experimental and numerical study of flow and heat transfer in helium cooled divertor finger mock-up with sectorial extended surfaces", S. Rimza, S. Khirwadkar, K. Velusamy, *Applied Thermal Engineering (Elsevier)*, 2015, 82, 390–402.
4. "Numerical studies on helium cooled divertor finger mock up with sectorial extended surfaces", S. Rimza, K. Satpathy, S. Khirwadkar, K. Velusamy, *Fusion Engineering and Design (Elsevier),* 2014, 89, 2647–2658.

Communicated:

1. "Development of Heat Sink Concept for Near Term Fusion Power Plant Divertor", S. Rimza, S. Khirwadkar, K. Velusamy, Journal of physics (IOP).

To be Communicated:

1. Effect of nozzle shapes, arrangement and nozzle diameter on the thermal performance of helium cooled divertor heat sink concept" S. Rimza, S. Khirwadkar, K. Velusamy, Nuclear Engineering and Technology.

Conferences:

1. "Development of heat sink concept for near-term fusion power plant divertor", S. Rimza, S.S. Khirwadkar, K. Velusamy, , 10th Asia Plasma & Fusion Association Conference (APFA - 2015), Gandhinagar, INDIA, 14th -18th Dec 2015.
2. "Numerical studies on helium cooled divertor finger mock-up with sectorial extended surfaces", S. Rimza, K. Satpathy, S.S. Khirwadkar, K. Velusamy, , 41th International Conference on Fluid Mechanics and Fluid Power, IIT-Kanpur, INDIA, 12th -14th Dec 2014.
3. "Studies on divertor cooling finger of helium mock-up through CFD approach", S. Rimza, K. Satpathy, S. Khirwadkar, K. Velusamy, Proceeding of the International Workshop on New Horizons in Nuclear Reactor Thermal Hydraulics and Safety, BARC, Mumbai, INDIA, 13th - 15th Jan 2014.
4. "DEMO Divertor Readiness Gaps and Needed R&D", S.S. Khirwadkar, V. Menon, S. Rimza et al., 1st IAEA DEMO programme workshop , University of California, Los Angeles, California, USA, 15th -18th Oct 2012.

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65. Name : **C.S. Reddy Bhoomireddy**
Enrolment No. : ENGG01201104004
Date of Award of degree : 14.07.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Recovery times of a spark gap with high pressure gases as insulation suitable for repetitive applications.

Abstract

Spark gap switch is the key element in any pulsed power system, which directly determines the pulse repetitive frequency of the system. The estimation of the recovery time is an important issue for the repetitive pulse power systems.In order to understand the dominant factors involved ingaseous spark gap recovery, investigations are being made todetermine the recovery holdoff voltage as a function of timefor smallspark gaps. Thework described herein is directed toward high-pressure gapswhich are over-volted by impulses. To obtain recovery information,two high-voltage pulses are applied to a spark gap with avariable time delay between them. The first pulse is used toover-volt and break down the gap, and the second pulse is usedto determine the voltage hold-off (recovery) of the gap after atime delay. A pulse transformer based double pulse generator capable of generating 40 kV peak pulses with rise time of 300ns and 1.5μs FWHM and with a delay of 1 ms -1s was developed, which is used for spark gap recovery studies. The work involves the estimation of recovery characteristics by varying the gap distance, gas medium, pressure level, electrode shape and size, pulse shape and size and also the impedance in the spark gap.An intermediate plateu is observed in all spark gap recovery curves. Shorter gaps in length are recovering faster than longer gaps.An increase in the output impedance resulted in a decrease in the time taken for recovery of spark gap.

Furthermore, a two-dimensional axisymmetric computational model of spark gap recovery is presented to provide a better understanding of the dynamics of the recovery process.These results illustrate the voltage recovery of a spark gap is significantly slower compared to the gas density recovery.Finally, atheoriticalmethod has been proposed to estimate the effect of spark gap electrode temperature rise and decay on repetition rate of spark gap.By using this method, the behavior of copper and stainless steel materials were studied.

Publications

Journal

1. C.S.Reddy, Archana Sharma and K.C. Mittal, "*Experimental Investigations of Pulse Charged Spark Gap Recovery Times and Influencing Factors*," *IEEE Transactions on Plasma Science,* Vol.44, Issue 3, pp. 331-337, 2016.
2. C.S.Reddy, A. S Patel, P. Naresh, Archana Sharma and K.C. Mittal, "*Experimental investigations of argon spark gap recovery times by developing a high voltage double pulse generator.*"*Review of Scientific Instruments*85, 064703 (2014); DOI: 10.1063/1.4883997.Published by the AIP Publishing LLC.
3. C.S.Reddy, Archana Sharma and K.C. Mittal, "*Recovery Analysis of Sparkgap by Anode Temperature Decay method for Different Materials.*"*International Journal of Applied Electromagetics and Mechanics*,Vol47, pp 643-651, 2015.Published by IOP press.
4. C.S.Reddy, Archana Sharma and K.C. Mittal "*Recovery study of Argon spark gap after Breakdown.*" *IEEE Transactions on Plasma Science.* (Under minor review).

International Conferences

1. C.S.Reddy,A.K Tak,Archana Sharma and K.C. Mittal, "*Computational modeling of spark gap density recovery after breakdown" IEEE International symposium On Discharges and Electrical Insulation in Vacuum (ISDEIV) -2014.*
2. C.S.Reddy, P. Naresh,Archana Sharma and K.C. Mittal, "*Voltage Recovery Characteristics of Spark gap using Repetitive Pulse Power System" IEEE International Power Modulator and High Voltage Conference (IPMHVC)*, USA, June-2014.
3. C.S.Reddy, P. Naresh,Archana Sharma and K.C. Mittal, "*Spark Gap Discharge Properties Measured by Optical Emission Spectroscopy"IEEE International Power Modulator and High Voltage Conference (IPMHVC)*, USA, June-2014.
4. C.S.Reddy, S.Mitra, S. B. Umbarkar,Archana Sharmaand K.C.Mittal, "*Optimisation of Sequential Triggering Delay in a Coaxial Fast Erecting MARX Generator"IEEE Pulse power conference,*USA, June-2013.
5. C.S.Reddy, S. B. Umbarkar,Archana Sharmaand K.C.Mittal,"*3D Particle in cell simulations of spark gap Discharge using Argon gas as dielectric medium"IEEE Pulse power conference,* USA, June-2013.
6. C.S.Reddy,S.V.Tewari,Archana Sharma,K.C.Mittal and D.P.Chakravarthy,"*Effect of anode temperature rise and decay on recovery times of sparkgaps"IEEE 4th Euro-Asian Pulsed Power Conference (EAPPC/BEAMS 2012)* Karlsruhe, Germany, October-2012.

66. Name : **Ekta Rani**
Enrolment No. : PHYS03201004008
Date of Award of degree : 14.07.16
Constituent Institute : Raja Ramanna Centre for Advanced Technology,
Title : Study Of Semiconductor Nanocomposites Using Raman And Afm Mapping.

Abstract

Materials at nanoscale show unique properties due to their large surface-to-volume ratio and or quantum size effects. In addition, studies at nanoscale are important for miniaturization of devices with improved performances. Recently, there have been large number of studies on a new class of materials - known as nanocomposites (NCps) in which nanostructures are embedded into a processable matrix that can be either ceramic or polymer [1,2]. These NCps find applications in variety of devices e.g. photovoltaic [3,4], optoelectronic [5], etc. It is therefore essential to synthesize and characterize the NCps, to ensure the reproducibility of the process that can be scaled-up. The properties of NCps depend not only on the individual components, but also on their interaction and morphology [2]. Therefore, to have desired control on growth of a NCp, it is imperative to understand the characteristic of individual component in the presence of other and the formation mechanism(s) of NCps. Raman spectroscopy is an excellent non-contact, non-destructive optical tool to study size, crystalline quality, stress, surface/interface, structure, phase transition, effect of doping etc. of a semiconductor nanostructure. Therefore, spatial variation of local bonding environment of semiconductor nanocrystals (NCs) in a matrix can be effectively probed using Raman mapping. *The motivation of this thesis work was to use Raman spectroscopy for the investigation of two specially chosen class of NCps: (i) Si-SiO2 (ceramic matrix) and ii) CdS-polyvinyl pyrrolidone (PVP: polymer matrix) NCps.* In the first case, an inorganic ceramic matrix is an oxide of the same semiconductor, whereas in the second case, organic matrix provides a completely heterogeneous NCp. The interactions between the semiconductor NCs and a matrix are expected to be quite different in these two cases. The results obtained using Raman spectroscopy had been supported by other techniques, such as, atomic force microscopy (AFM), vi X-ray diffraction and X-ray photoelectron spect

Publications

Journal

1. On red-shift of UV Photoluminescence with decreasing size of Si nanoparticles embedded in SiO2 matrix grown by pulsed laser deposition; Amita Chaturvedi, M. P. Joshi, Ekta Rani, Alka Ingale, L. M. Kukreja and A. K. Srivastava, J. of Luminescence (2014) 154, 178–184.
2. Correlation of size and oxygen bonding at the interface of Si nanocrystal in Si-SiO2 nanocomposite: A Raman mapping study; Ekta Rani, Alka A. Ingale, A. Chaturvedi, C. Kamal, D. M. Phase, M. P. Joshi, A. Chakrabarti, A. Banerjee and L. M. Kukreja, J. of Raman Spectroscopy (2016) 47, 457-467
3. Insight into one-step growth of nearly monodispersive CdS nanocrystals embedded in polyvinyl pyrrolidone spheres; Ekta Rani, Rahul Aggarwal, Alka A Ingale, K. Bapna, C. Mukherjee, M. K. Singh, P. Tiwari and A. K. Srivastava, J. of Materials Science (2016) 51, 1581-1590.
4. Resonance Raman mapping as a tool to monitor and manipulate Si nanocrystals in Si-SiO2 nanocomposite; Ekta Rani, Alka A. Ingale, A. Chaturvedi, M. P. Joshi and L. M. Kukreja, Appl. Phys. Lett. (2015) 107, 163112.
5. Corroboration of Raman and AFM mapping to study Si nanocrystals embedded in SiO2;Ekta Rani, Alka A. Ingale, A. Chaturvedi, M. P. Joshi and L. M. Kukreja J. of Alloys and Compounds (2016) 672, 403-412

Presented in International Conferences:

1. Insight into growth of CdS-PVP NCps using Raman and PL mapping. **Ekta Rani**, Alka A. Ingale, Rahul Aggarwal, **Proc. of International conference on Raman spectroscopy** (ICORS) India, August 2012.

2. Probing interface of Si nanocrystals in Si-SiO2 NCp using Raman mapping. **Ekta Rani**, Alka A. Ingale, A. Chaturvedi, M. P. Joshi and L. M. Kukreja, **Proc. of International conference on nano science and technology** (ICONSAT) India, March 2014 **has received Best poster Award.**

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67. Name	:	**Anuraag Misra**
Enrolment No.	:	ENGG04201004001
Date of Award of degree	:	14.07.16
Constituent Institute	:	Variable Energy Cyclotron Centre
Title	:	Studies on generation and characterization of high current beams from microwave ion source.

Abstract

Department of Atomic Energy is considering a high intensity accelerator to deliver a 1 GeV, 10 mA proton beam for Accelerator Driven Subcritical System. As a first step towards the development of this system, a R&D program is underway at Variable Energy Cyclotron Centre for the development of 2.45 GHz proton source along with a low energy beam transport system (LEBT) to study the production and transport of proton beam in the range of (10-15) mA at ~75 keV energy. At present, the ion source is operational and produces a 12 mA beam current for 400 W of microwave power. A beam current of ~ 6 mA through a 10 mm diameter aperture has been transported to three meters from the ion source. In this thesis, we report the results of a detailed study investigating the effect of variation in different parameters of the ion source, like, for instance, microwave power, magnetic field profile, gas pressure, etc. on the performance of ion source. It is demonstrated that these parameters have significant impact on the extracted beam current and proton fraction. This thesis also presents a unique analytical method for the design of binomial matching transformer. A comparison of the results obtained from analytical method and finite element method simulations, shows that they are in good agreement. It is demonstrated that usage of optimum matching transformer improves the performance of microwave ion source. The maximum beam transmission and the beam quality in LEBT are limited by the space charge effects of high current proton beam. Thus, these effects must be mitigated by space charge compensation (SCC). The compensated beam should also be characterized before injecting it into the cyclotron. This thesis report the results of SCC in a 75 keV, 5mA proton beam. The SCC is realized by injection of Ne gas into the beam line. It is shown that RMS beam size reduces by ~ 34 % with the SCC. A residual gas fluorescence monitor was used to measure the beam profile. The solenoid scan with sigma matrix method was used to determine the normalized RMS beam emittance. It is measured to be of 0.05 mm-mrad.

Publications

Journal

1. V.S. Pandit, P.Sing.Babu, A. Goswami, S. Srivastava, A. Misra, M. Chatterjee, P.Y. Nabhiraj, et.al., "Development of microwave ion source and low energy beam transport system for high current cyclotron", Nucl. Instrum. Methods Phys. Res. B 317, 434 (2013).

2. Anuraag Misra and V.S. Pandit, “Studies on the coupling transformer to improve the performance of microwave ion source", Rev. Sci. Instrum. 85 063301 (2014).
3. Anuraag Misra, A. Goswami, P.Sing. Babu, S. Srivastava and V.S. Pandit, “Studies on space charge neutralization and emittance measurement of beam from microwave ion source”, Rev. Sci. Instrum. 86 113301 (2015).

Conference Publications:-

1. Anuraag Misra, V.S. Pandit, G. Pal, H.K. Pandey, “Design and development of a double ridged waveguide for a 2.45 GHz microwave ion source”, InPAC-2011 , New Delhi.
2. Anuraag Misra , V.S. Pandit and G. Pal, “Design of high current bunching system and fast faraday cup for high current LEBT at VECC “, Proceedings of International Workshop on accelerator-driven subcritical systems and thorium utilization, 2011, Mumbai.
3. V.S. Pandit, G. Pal, S.K. Thakur, P.S. Babu, A. Goswami, M. Chatterjee, R.C. Yadav, S. Srivastava, S. Bhattacharya, S. Roy, C. Nandi and A. Misra “Microwave Ion source and injection system for a high current compact cyclotron”, Proceedings of International Workshop on accelerator-driven subcritical systems and thorium utilization, 2011, Mumbai.
4. V.S. Pandit, R.C. Yadav, G. Pal, C. Nandi, A. Goswami, P.S. Babu, S. Srivastava, A. Misra, “Vaccum system of the ion source and injection line of a high current compact cyclotron.”, Journal of Physics Conference Series 11/2012; 390(1): 2066.
5. Anuraag Misra, S. Srivastava, V.S. Pandit, “Effect of coupling transformer on the performance of microwave ion source: simulation and experiment”, Proceedings of Indian National Particle Accelerator Conference 2013, pp. 317.
6. Anuraag Misra, P.Sing. Babu, A. Goswami, S. Srivastava, V.S. Pandit, “Characterization of high intensity beam from 2.45 GHz microwave ion source”, Proceedings of Indian National Particle Accelerator Conference 2013, pp. 314.
7. Anuraag Misra and V.S. Pandit, “Development of high current microwave feeding system for high current ion source”, Proceedings of IEEE Applied Electromagnetics Conference 2013, 978-1-4799-3267-2/13.

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68. Name : **Deepak Kumar Sahoo**
Enrolment No. : CHEM01200904002
Date of Award of degree : 14.07.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Study On Electrodeposition Of Light Rare Earth Metals And Alloys From Molten Chloride Electrolytes.

Abstract

Rare Earth metals find extensive uses in fields like in the production of clean energy, in electronic devices, aerospace and defense applications.To meet the growing demand of rare earth based materials, better metallurgical technologies are required for the synthesis and engineering scale production of rare earth metals and their alloys in an efficient and economical way. The production of rare metals by molten salt electrolysis has an important role because large scale production of rare earth metals by this route is more economic compared to other existing methods.The present investigation was undertaken to study the preparation of four light rare earth metals i.e. La, Ce, Pr and Nd and some of their alloys i.e. La-Mg and Nd-Fe by molten salt electrolysis.Rare earth chlorides which are used as electrolytic precursor material in synthesis of rare earth metals and alloys are highly hygroscopic in nature. In this study, extensive work has been carried out to find a suitable and efficient way of dehydration of rare earth chloride hydrates which is extremely important for the success of electro-winning process.Studies related to electro-kinetic parameters

such as electron transfer co-efficient, electron transfer rate constant, diffusion co-efficient have been carried out to draw more insight into the process.Process parameters like temperature of operation, electrolytic composition and cathode current densities have been standardized to get maximum current efficiency and yield in the bulk deposition of metal.Electro-deposition of two alloys namely La-Mg and Nd-Fe were studied by co-deposition and consumable cathode technique respectively. The electrochemistry and mechanism of the deposition process were studied by cyclic voltammetry, and open circuit potentiometry. The effects of various process parameters such as composition of electrolyte in the bath, temperature of electrolysis and cathode current density on current efficiency have been investigated to get maximum current efficiency in both the cases.

Publications

Journal

1- Current efficiency in electro-winning of lanthanum and cerium metals from molten chloride electrolytes D.K.Sahoo, H.Singh, Krishnamurthy, *Rare Metals* 32-3 (2013) 305-311.
2- Determination of thermodynamic stability of lanthanum chloride hydrates ($LaCl_3 \cdot xH_2O$) by dynamic transpiration method by D.K. Sahoo, R. Mishra, H. Singh, N. Krishnamurthy, *Journal of Alloys and Compounds* 588 (2014) 578–584.
3- Electrochemical deposition of La-Mg alloys in $LaCl_3$-$MgCl_2$-KCl system with molten salt electrolysis process by D.K.Sahoo, H.Singh, N.Krishnamurthy, *J. Min. Metall. Sect. B-Metall.* 50 (2) B (2014) 109 – 114.
4- Electrochemical properties of Ce (III) in equimolar mixture of LiCl-KCl and NaCl-KCl molten salts by D.K.Sahoo, A.K.Satpati, N.Krishnamurthy. *RSC Adv*., 5 (2015) 33163–33170.

Conference publications

1- Electrodeposition of light rare earth metals in fused chloride bath “D.K.Sahoo, Sanjay Kumar, A Mukherjee,N.Krishnamurthy”Proceedings of international symposium on environmental management of mining and minerals based industries, August 18-20 (2010) ,Bhubaneswar, pp-51-58.
2- Determination of vapor pressure of H_2O over $LaCl_3.7H_2O$ and intermediate compounds by dynamic transpiration method; D.K.Sahoo, R.Mishra, D Das and N Krishnamurthy; 18th International symposium on thermal analysis, Feb.2-4 (2012), Anushaktinagar, Mumbai pp 67-69.
3- Study on electrodeposition of La-Mg alloys in chloride system with molten salt electrolysis process, D.K.Sahoo, H.Singh, N.Krishnamurthy, National conference on Rare earths and uranium processing & utilizations (REPUT-2014).May 2-4 (2014), Anushaktinagar, Mumbai-400094.p-45.
4- Electrochemical behavior of Pr (III) In NaCl-KCl molten salt, D.K.Sahoo,R.Mishra,EUCHEM Conference on Molten Salts AND Ionic Liquids,3rd -8th July 2016,Austria,Vienna.

69. Name : **Rajender Kumar Bhatia**
Enrolment No. : PHYS01201204015
Date of Award of degree : 14.07.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Development Of Magnetic Sector Mass Spectrometers For Isotopic Ratio Analysis.

Abstract

Mass spectrometry is widely used analytical technique for a variety of applications viz. precise isotopic ratio measurement, trace elemental analysis and compositional analysis of materials as well as characterization of bio-organic molecules etc [1]. Mass spectrometers find application in different fields as nuclear, geochronology, biology, material science, pharmaceutical industry, petrochemical industry, hydrology, environmental science, geology, planetary science etc. There are different types of mass spectrometers based on ion source design, analyzer for separation of ions based on charge/mass and detectors [2-4]. A specific design is selected based on the application. To mention a few– magnetic sector based mass spectrometers are used for the precise isotopic ratio measurements [5], a mass spectrometer with high ionization efficiency like inductively coupled plasma [6] or glow discharge mass spectrometer [7] is employed for trace elemental detection, a quadrupole based mass spectrometer is used for the compositional analysis of mixture of gases [8], and for the characterization of bio organic molecules mass spectrometers with soft ionization techniques like matrix assisted laser desorption ionization (MALDI) [9] and electro spray ionization (ESI) are employed [10,11].The work presented in the thesis is mainly concerned with the developments carried out to improve the performance of a thermal ionization mass spectrometer (TIMS) which is a magnetic sector based mass spectrometer. These would also be useful for most of other magnetic sector based mass spectrometers. TIMS is used for the precise isotopic ratio measurement of elements for application in various fields like nuclear, geochronology, environmental science etc. The magnetic sector analyzer has unique advantage of simultaneous measurements of ions of different mass to charge ratio thereby eliminating possible errors due to fluctuations in the ion beam due to any parametric variations in ion source or analyser. It can be used in combination with variety of ion sources like electron impact ion source, thermal ionization source, inductively coupled plasma source etc. The work incorporates design, development, testing and evaluation of various sub systems of TIMS and studies to improve the performance in terms of precision and sensitivity of TIMS [12]. The thesis has been divided into seven chapters with first two chapter giving general introduction to mass spectrometers and basic design of TIMS used in present studies. Chapters 3 to 6 present studies made for improvement in different components of this basic design and last chapter presents summary of the thesis and scope for further work. The improvements carried out are: (a) ion source design by insertion and modification of electrode plates to improve sensitivity, (b) design modification of magnetic sector analyzer by addition of shims to result in focal plane normal to principal beam axis, (c) development of zoom optics to result in mechanical simplicity of collector system and (d) studies on Faraday cup for improvement in collection efficiency. These will be discussed in later chapters. A summary of different chapters is given in the following.

Publications

Journal

1. “Rotation of focal plane of magnetic analyzer in an isotope ratio mass spectrometer using curved shims”, Rajender K. Bhatia, Yogesh Kumar, K.Prathap Reddy, V.K.Yadav, E.Ravisankar, T.K.Saha, V.Nataraju, V.K.Handu, *International Journal of Mass Spectrometry*, 2012, *313*, 36-40.
2. “A Novel Variable dispersion zoom optics for isotope ratio sector field mass spectrometer”, Rajender K. Bhatia, Varun K.Yadav, Vilas M. Mahadeshwar, Milind M. Gulhane, E.Ravisankar, T.K.Saha, V.Nataraju, S.K.Gupta, *International Journal of Mass Spectrometry,* 2013*, 339-340,* 39-44

3. "Improved Faraday collector for magnetic sector mass spectrometers", Rajender K. Bhatia, Varun K.Yadav, Yogesh Kumar, Babu R. Gonde, E.Ravisankar, T.K.Saha, V.Nataraju and S.K.Gupta, *International Journal of Mass Spectrometry,* 2015*, 393,* 58-62

Conferences

1. "Development of a Novel Variable Dispersion Zoom Optics for Magnetic Sector Mass Spectrometer" Rajender K Bhatia, Varun K. Yadav, Vilas M Mahadeshwar, Milind M Gulhane, E.Ravisankar, T.K.Saha, V.Nataraju and S.K.Gupta, *12th ISMAS TRICON*, 2013, 206-207
2. "Experiments on a new Faraday cup design in an in-house built magnetic sector mass spectrometer" R.K.Bhatia, Yogesh Kumar, Varun K Yadav, Rabi Datta, E Ravisankar, T.K.Saha and V. Nataraju, *28th ISMAS-WS*, 2014, 224-227
3. "Studies on design modifications in a Thermal ionization source for improved sensitivity" Arkadip Bhasak, R.K.Bhatia, Varun K Yadav, Madhavi Sharma, Yogesh Kumar, E.Ravisankar and V.Nataraju , *28th ISMAS-WS*, 2014, 161-165
4. "An electron impact ion source as a switch-over option for TIMS" R.K.Bhatia, Babu R Gonde, V.K.Yadav, M.M.Gulhane, E.Ravisankar, T.K.Saha and V.Nataraju, *29th ISMAS international symposium on mass spectrometry*, 2015, 158-159.

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70. Name : **Tanmoy Modak**
Enrolment No. : PHYS10201004001
Date of Award of degree : 20.07.16
Constituent Institute : Institute of Mathematical Sciences,
Title : Study Of Spin, Parity And Couplings Of A Bosonic Resonance At Colliders.

Abstract

In this thesis we outline a step by step methodology to determine the spin, parity and couplings of the 125 GeV resonance (H) discovered at LHC. We study experimentally clean "gold-plated" decay mode of H, where it decays to two Z bosons followed by subsequent decays of the two Z bosons into four non-identical charged leptons. Since the resonance is found to be decaying into di-photon channel i.e. $H \rightarrow \gamma\gamma$ it can not be a Spin-1 particle, prohibited by Landau-Yang's theorem. We begin with writing down the most general Lorentz and gauge invariant vertex factor of H for both the spin possibilities i.e.Spin-0 and Spin-2. We then derive three uniangular distributions in terms of severalangular asymmetries. These angular asymmetries have definite parity signatures and are orthogonal to each other. Thus they can be measured independently. We find that these asymmetries have different characteristics for a Spin-0 resonance compared to a Spin-2 resonance and can be used to determine the spin of H. After identifying the spin, these asymmetries can be used to study the parity of H. We corroborate our methodology by numerical analysis. In SM the value of the HZZ couplings are uniquely predicted. After the discovery of H, it is esstial to study the HZZ couplings precisely to confirm its SM nature. Although 8 TeV run indicates H to be a Spin-0 resonance with even parity, a considerable amount of CP-odd admixture is still possible. We show in this thesis, how one can precisely probe CP-odd admixtures of HZZ couplings at 14 TeV LHC run for two different luminosities. The direct measurement of the absolute values of the couplings are beyond the scope of the LHC which requires a precise measurement of the partial rate. We show how using angular asymmetries one can obtain the ratios of couplings and the relative phases between them. This precision measurement of couplings have the potential to find New Physics beyond SM.Almost all GUT motivated theories predict the existence of a massive Z' boson which is Spin-1 boson. Finding such particle would give us unique understanding of the physics beyond the Standard Model. In this thesis we show how three uniangular distributions can be used to probe the spin, parity and couplings of a Z' via gold-plated decay mode where it decays to two Z bosons. A numerical analysis is also performed to show the applicability of our methodology for experimental study.

Finally we have combined these results and presented a step by step methodology to uniquely determine the spin, parity and couplings of a new resonance via gold-plated decay mode with any arbitrary mass. Thus it would not be a overstatement that uniangular distributions have the potential to confirm the true characteristic of bosonic a resonance.

Publications

Journal

1. Inferring the nature of the boson at 125-126 GeVArjun Menon, Tanmoy Modak, Dibyakrupa Sahoo, Rahul Sinhaand Hai-Yang Cheng PHYSICAL REVIEW D 89, 095021 (2014)arXiv:1301.5404[hep-ph]
2. Disentangling the Spin-Parity of a Resonance via the Gold-Plated Decay ModeTanmoy Modak, Dibyakrupa Sahoo, Rahul Sinha, Hai-Yang Cheng and T.C. Yuan Chinese Physics C Vol. 40, No. 3 (2016) 033002 arXiv:1411.2210[hep-ph]

3. On probing Higgs couplings in H → Z V decays Tanmoy Modak and Rahul Srivastava arXiv:1411.2210[hep-ph]
4. Probing Higgs couplings at LHC and beyond Biplob Bhattacherjee , Tanmoy Modak, Sunando Kumar Patra and Rahul Sinha arXiv:1503.08924[hep-ph]
5. 750 GeV Diphoton excess from Gauged B–L Symmetry Tanmoy Modak, Soumya Sadhukhan and Rahul Srivastava Physics Letters B 756 (2016) 405–412 arXiv:1601.00836[hep-ph]

Conference Proceedings :

1. Study of the Spin-Parity of a Resonance via the Gold-Plated Decay Mode Tanmoy Modak Published in Springer Proc.Phys. 174 (2016) 571-576

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71. Name : **Arindam Roy**
Enrolment No. : PHYS04201004007
Date of Award of degree : 20.07.16
Constituent Institute : Variable Energy Cyclotron Centre
Title : Probing matter created at RHIC heavy-ion collisions by di-muons and photons at mid and forward rapidities

Abstract

In recent times, ionic liquids (ILs) have attracted considerable attention both from academia and industry mainly due to their attractive physicochemical properties and their use in several applications.[1,2] Geminal dicationic ionic liquids (DILs), having two unit positive charge, are expected to be advantageous over traditional monocationic ionic liquids (MILs) as DILs have been shown to possess superior physicochemical properties in contrast to MILs.[3,4] In this regard, studies with an aim to understand the structure-dynamics correlation in these specialized media are of extreme importance for effective utilization of these systems. The present thesis is focused to understand the kinship among structure, intermolecular interactions and dynamics through solute and solvent dynamics study in mono and dicationic RTILs by employing steady-state and time-resolved fluorescence as well as Nuclear Magnetic Resonance (NMR) studies.

Publications

Journal

2. “Calibration and performance of the STAR Muon Telescope Detector using cosmic rays"Yang C. et al for the STAR CollaborationNucl.Instrum.Meth. A762 (2014) 1 , [arXiv:1402.1078]

3. “Development of Multi-gap Resistive Plate Chamber (MRPC) for medical imaging"A. Banerjee, A. Roy, S. Biswas, S. Chattopadhyay, G. Das, S. Pal.
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4. “Performance simulation of a MRPC-based PET Imaging System"A. Roy,A. Banerjee, S. Biswas, S. Chattopadhyay, G. Das, S. Saha.\2014 JINST 9 C10030

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72. Name : **S. Mahadevan**
Enrolment No. : ENGG02200804019
Date of Award of degree : 20.07.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : X-ray diffraction based characterization of ageing behaviour of precipitation hardenable steels.

Abstract

This study is intended to demonstrate the applicability of using the parameters derived from analysis of X-ray diffraction (XRD) profiles for characterizing the ageing behaviour of two precipitate strengthened alloys, viz., 17-4 PH steel and M250 grade maraging steel. These two materials, under solutionized condition, are known to have high dislocation density. On ageing, hardness increases due to precipitation. While coherent precipitates increase the microstrain in the matrix, annihilation of dislocations reduces the microstrain. The XRD peak profile broadens, when the crystallite size is small or when the material contains lattice defects. When the crystallite shape or strain is anisotropic, the broadening does not change linearly with diffraction angle. To account for the anisotropic strain broadening, Ungár and Borbély proposed a modified Williamson-Hall (mWH) plot and a modified Warren-Averbach (mWA) analysis, which are based on the contrast caused by dislocations to profile broadening. These two approaches are used for estimating the changes in microstrain and crystallite size variation due to precipitation and microstructural changes that occur during ageing of these two steels. An approach is proposed to determine the precipitate fraction from changes in lattice parameter by using the atomic volume occupied by each of the alloying elements. The precipitate fraction estimated by this approach is compared with that obtained from changes in hardness. In 17-4 PH steel, the changes in crystallite size were found to be consistent with the microstructural investigations carried out with scanning electron microscope. The Avrami exponent and the activation energy for the precipitation process have been determined from hardness measurements and they are found to compare well with published literature. The changes in hardness in the overaged regime and microstrain in the incoherent regime have been uniquely linked with the tempering parameter which links the temperature and duration of ageing. In maraging steel, the root mean square strain as a function of column length has been evaluated from modified WA analysis. The changes in microstrain at shorter column lengths are linked to dislocation annihilation behaviour. The similarity of the long range strain with the microstrain estimated from the modified WH approach shows the effect of precipitates. The increase in strength on ageing of 17-4 PH steel has been attributed to the coherency strengthening arising from the Cu precipitates and the modulus strengthening arising due to the difference in shear modulus of the precipitates and that of the matrix. In maraging steel, the strengthening has been attributed to the order strengthening which arises due to the formation of Ni_3Ti during initial ageing. The various precipitate strengthening mechanisms are theoretically estimated from experimentally determined microstrain and precipitate fraction along with calculated precipitate radius. The measured hardness is uniquely linked and compared to the precipitate strengthening and grain boundary strengthening contributions using a new 3-dimensional planar equation. The above proposed approach clearly shows that coherency strengthening, modulus strengthening and grain boundary strengthening act in tandem and result in improved strength of 17-4 PH steel. In maraging steel, in addition to coherency and modulus strengthening, order strengthening acts along with grain boundary strengthening to contribute to the observed increase in yield strength. The Hall-Petch constant determined from the planar fit is in agreement with literature. This study clearly shows that the parameters estimated from XRD profile analysis, like lattice parameter, microstrain, crystallite size and dislocation density can be used to understand the microstructural changes that occurs during ageing and enables in-depth understanding of the strengthening behaviour of these two precipitation hardenable steels.

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2. Anil Kumar. Soni, B. Purna Chandra Rao, S. Mahadevan and S. Thirunavukkarasu, ‘A study on the scan plans for rapid eddy current non-destructive evaluation’, Journal of Nondestructive Evaluation (Under Review).
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4. Anil Kumar. Soni, S. Thirunavukkarasu, B. Sasi, B. Purna Chandra Rao, T. Jayakumar, ‘Development of a high sensitive eddy current instrument for detection of sub-surface defects in stainless steel plates’, Insight-Non-Destructive Testing & Condition Monitoring Vol. 57, No. 9, September 2015, pp. 508-512, DOI: 10.1784/insi.2015.57.9.508.
5. S. Thirunavukkarasu, B. Purna Chandra Rao, Anil Kumar Soni, S. Shuaib Ahmed, T. Jayakumar, ‘Comparative performance of image fusion methodologies in eddy current testing’, Research Journal of Applied Sciences, Engineering and Technology, Vol. 4, No. 24, 2012, pp. 5548-5551.

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1. Anil Kumar Soni, S Shuaib Ahmed, S. Thirunavukkarasu, B. Purna Chandra Rao and T Jayakumar, ‘Multi-Sensor Image Fusion for Enhanced Detection of Sub-Surface Defects by Eddy Current Testing’, Presented during the 14th Asia Pacific Conference on Non-destructive Testing, Mumbai, 2013.
2. Anil Kumar Soni, B. Purna Chandra Rao, B. Sasi, Saji Jacob George, T Jayakumar, ‘Development of a Low Frequency Eddy Current Instrument for Non-destructive Evaluation’, Presented during the National Symposium on Instrumentation (NSI-38), Hubli, 2013.

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73. Name : **Kamakshya Prasad Modak**
Enrolment No. : PHYS05201004008
Date of Award of degree : 03.08.16
Constituent Institute : Saha Institute of Nuclear Physics,
Title : Investigating Some Aspects of Dark Matter Indirect Detection Using different Dark Matter Particle Physics Models

Abstract

The research done in my Ph.D. thesis mainly relates to simple particle physics models of Dark Matter that can be constructed by simple extensions of the Standard Model (SM) and various aspects of indirect detection signatures for such dark matter particles are extensively studied. Dark matter represents an unknown, non-luminous form of matter whose presence is inferred only via gravitational effects on galaxies and stars. The presence of dark matter is now well established by various cosmological and astrophysical evidences. Observations such as WMAP or PLANCK suggest that around ~26.8% of the total content of the Universe is constituted by this invisible form of matter. The indirect detection of dark matter involves detecting the particles (and their subsequent decays) or photons produced due to dark matter annihilations. These annihilation products can be fermions and γ photons etc. The dark matter particles, if trapped in considerable amount by the gravity of a massive body like sun or galactic centre, can annihilate there to produce these particles. Study of such photons and fermions such as neutrinos thus throw light on the nature of galactic dark matter as well as the nature of the galactic dark matter halo profile.Throughout the analyses performed in this Ph.D. thesis, I have considered direct γ-ray emission from the final state particles of dark matter annihilations, where γ-ray emits from the final charged leptons or from neutral pion decay after hadronisation. In this thesis work, I have calculated those gamma ray fluxes from the galactic centre as also from other places in galactic dark matter halo along the line of sight around the galactic centre. Different satellite-borne and ground-based experiments such as Fermi-LAT that looks for extra terrestrial gamma signals have reported the observance of excess gamma ray signals in the direction of galactic centre in different energy regions. Experiments such as Fermi-LAT, HESS etc. can detect very high energy gamma rays from the galactic centre, which has no known astrophysical origin. To this end some particle physics models for dark matter beyond the SM of particle physics are proposed and some other known models are explored in detail in this thesis in order to study the phenomenology of indirect detection of dark matter through gamma rays. These models include two-component singlet scalar dark matter model (the scalar sector of SM is enlarged with the addition of two SM singlet real scalars), an inert Higgs doublet model (SM is extended with a Higgs-like scalar doublet with no vacuum expectation value), minimal anomaly mediated supersymmetry breaking (mAMSB) model (dynamical or spontaneous supersymmetry breaking propagates from hidden sector to observed sector via loop generated superconformal anomaly and neutralino is the candidate for dark matter), radiative neutrino mass model (three right-handed singlet neutrinos and one Higgs-like scalar doublet are added to the SM). The detailed theoretical aspects of such models are widely explored and developed in cases. Also the phenomenologies of all these models are elaborately studied in order to confront both the direct as well as the indirect detection signatures of dark matter. The theoretical frameworks for the unresolved emission of excess gamma rays from Galactic Centre, Fermi Bubble, galactic dark matter halo region, dwarf spheroidal galaxies as well as from extragalactic sources are well explored in the light of those well-motivated particle physics models for dark matter where possible indirect signatures of dark matter are extensively computed for those models and compared with the available observational results. Moreover, the anomalous X-ray lines from the observation of Andromeda galaxy and 73 other galaxy clusters are confronted with the simple leptophilic model (radiative neutrino mass model) for dark matter.

Publications

Journal

1. “Gamma Ray and Neutrino Flux from Annihilation of Neutralino Dark Matter at Galactic Halo Region in mAMSB Model”,Kamakshya Prasad Modak, Debasish Majumdar,Journal of Physics G: Nuclear and Particle Physics, 40, 075201 (2013) [arXiv:1205.1996 [hep-ph]].

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5. “Confronting Galactic and Extragalactic γ-ray observed by Fermi-LAT with Annihilating Dark Matter in Inert Higgs Doublet Model”,Kamakshya Prasad Modak, Debasish Majumdar,Astrophysical Journal: Supplement Series, 219, no. 2, 37 (2015) [arXiv:1502.05682 [hep-ph]].

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74.	Name	:	**Mayanak Kumar Gupta**
	Enrolment No.	:	PHYS01201104011
	Date of Award of degree	:	03.08.16
	Constituent Institute	:	Bhabha Atomic Research Centre,
	Title	:	Thermodynamical Properties Of Functional Materials: Neutron Scattering And Lattice Dynamics Studies.

Abstract

The study of the vibrations of the atoms and molecules in a crystal is known as lattice dynamics. The temperature is interpreted in a material by its atomic vibrations. In order tohave a complete picture of crystalline materials, a deep understanding of lattice dynamics is required. The propagation of sound waves in crystals, Raman scattering of light and mabsorption of certain frequencies in the infra-red spectral region are some of the experimentalobservations of lattice dynamics. Without lattice dynamics it is not possible to explain various thermodynamical properties such as phase transitions, thermal conductivity, thermal expansion etc. Further, atomic vibrations also contribute to free energy in the form of entropy besides vibrational energy itself. In crystalline solids the motion of atoms are not random but follow certain rules defined by the neighboring atoms in the system. Incrystalline solids these well defined collective motions are quantized and are called as “phonons”. To characterize and understand the various properties in solid, it is highly desirable to study these phonons with the help of theoretical tools and inelastic-neutron/light scattering experiments. It is not always possible to perform experiment at high temperature and pressure conditions; in such cases, the simulation studies are used to predict the material properties under these extreme conditions. For this purpose, theoretical studies based on lattice dynamical methods are necessary for exploring the entire spectrum of thermal vibrations in crystals. The data obtained from experimental techniques are used to test and validate the theoretical methods. Once validated successfully, these methods may further be used to predict the thermodynamic properties at various thermodynamical conditions. The author has used the state of the art density functional theory methods to compute the total energy and forces, hence the phonons in entire Brillouin zone for various compounds. To validate the theoretical results, the author has also carried out inelastic neutron scattering experiments.The thesis consists of eight chapters. Application of density functional theory to a variety of oxide materials to understand the role of phonons in their functional properties of negative thermal expansion (NTE), multiferroicity or super-ionic conduction is presented. The motivation for studying the various compounds, details of the work done and the significance of the results obtained are given below in the brief description of various chapters.

Publications

Journal

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2. Suppression of antiferroelectric state in $NaNbO_3$ at high pressure from in situ neutron diffraction. S. K. Mishra, M. K. Gupta, R. Mittal, S. L. Chaplot, and Thomas Hansen Appl. Phys. Lett. 101, 242907 (2012).

3. Inelastic neutron scattering and ab-initio calculation of negative thermal expansion in Ag_2O M. K. Gupta, R. Mittal, S. L. Chaplot and S. Rols Physica B 407, 2146 (2012).

4. Negative thermal expansion in cubic ZrW_2O_8: Role of phonons in entire Brillouin zone from ab-inito calculations M. K. Gupta, R. Mittal and S. L. Chaplot Phys. Rev. B, 88, 014303 (2013).

5. Phonon dynamics and inelastic neutron scattering of sodium niobate S. K. Mishra, M. K. Gupta, R. Mittal, M. Zbiri, S. Rols, H. Schober, and S. L. Chaplot Phys. Rev. B 89, 184303 (2014).

6. Phonons, nature of bonding, and their relation to anomalous thermal expansion behavior of M_2O (M = Au, Ag, Cu).M. K. Gupta, R. Mittal, S. L. Chaplot, and S. Rols Journal of Applied Physics, 115, 093507 (2014).

7. Phonons lithium diffusion and thermodynamics of $LiMPO_4$ (M=Mn, Fe). Prabhatasree Goel, M. K. Gupta, R. Mittal, S. Rols, S. J. Patwe, S. N. Achary, A. K. Tyagi and S. L. Chaplot J. Mater. Chem. A, 2 14729 (2014).

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9. Spin-phonon coupling and high-temperature phase transition in multiferroic material $YMnO_3$. M. K. Gupta, R. Mittal, M. Zbiri, Neetika Sharma, S. Rols, H. Schober and S. L.ChaplotJ. Mater. Chem. C 3, 11717 (2015).

10. Phonons and stability of infinite-layer iron oxides $SrFeO_2$ and $CaFeO_2$.M. K. Gupta, R. Mittal, S. L. Chaplot, Cedric Tassel and Hiroshi Kageyama Solid State Communications 241, 43 (2016).

11. Spin-phonon coupling and high pressure phase transitions of $RMnO_3$ (R= Ca and Pr): An inelastic neutron scattering and first principle studies. S. K. Mishra, M. K. Gupta, R. Mittal, A. I. Kolesnikov and S. L. Chaplot Phys. Rev. B 93, 214306 (2016).

12. Lattice dynamics and thermal expansion behavior in metal cyanides, MCN(M=Cu,Ag, Au): Neutron inelastic scattering and first principles calculations. M. K. Gupta, Baltej Singh, R. Mittal, S. Rols and S. L. Chaplot Phys. Rev. B 93, 134307 (2016)

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75. Name : **Ashwani Kumar**
Enrolment No. : PHYS01201004008
Date of Award of degree : 03.08.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Design and development of protein crystallography beamline at Indus-2 synchrotron and structural studies of a bacterial prolidase and human PSP94.

Abstract

The thesis titled Design and development of protein crystallography beamline at Indus-2 synchrotron and structural studies of a bacterial prolidase and human PSP94 presents the design, construction and commissioning of protein crystallography beamline (PX-BL21). Latter part of the thesis deals with structural studies on prolidase and human PSP94 proteins. The PX-BL21 installed at 1.5 T bending magnet (BM) port

and has working energy range of 5 − 20 keV to access the absorption edges of heavy elements commonly used for phasing. This beamline is equipped with a single axis goniometer, Rayonix MX225 CCD detector, fluorescence detector, cryogenic sample cooler and automated sample changer. The thesis describes the ray tracing and heat load calculations in the context of beamline design and development. Thermal and structural analysis of beamline components has also been presented in the thesis. Also, thesis describes the hot alignment of beamline components in X-rays by using beam position monitors (BPMs). Finally, thesis describes the beamline optimization and its validation by collecting and solving crystal structure using SAD methods.Xaa-Pro dipeptidase or prolidase, specifically hydrolyzes the dipeptides with a prolyl residue in the carboxy terminus. The prolidase of 43 kDa size (XPD43 or PepQxc) from *Xanthomonas spp*., lacks strictly conserved tyrosine residue (equivalent to Tyr387 of Escherichia coli Aminpeptidase-P) that is suggested to be important in proton shuttle transfer, which is required for the catalysis in M24B (MEROPS) family. To study the role of conserved residues in prolidase family, a total of six (four native and two with R372A mutation) high resolution PepQxc crystal structures were determined. Further, the enzymatic studies have been carried out to analyze the substrate specificity of PepQxc towards the Xaa-Pro substrates. The crystal structure of native and R372A mutated PepQxc protein showed that the conserved residue Tyr which participates in hydrogen bond networking motif is replaced by Met residue. The loss in enzymatic activity in presence of phosphate ions has been explained on the basis of structure of PepQxc1-Mn and PepQxc1-Zn. PSP94 is one of the most abundant proteins from prostatic secretions and a primary constituent of human semen. PSP94 suppresses tumor growth and metastasis, and its expression gradually decreases during progression of the prostate cancer. The thesis presents the crystal structure of human PSP94 at 2.3 ˚A resolution. The structure shows that the amino and the carboxyl ends of the polypeptide chain are held in close proximity facing each other. Our studies further shows that dimers dissociate into monomers at acidic pH, possibly through distortion of the straight edge. Furthermore, based on several observations, we proposed that PSP94 binds to cysteine rich secretory proteins and immunoglobulin G through the same edge, which is involved in the formation of PSP94 dimeric interface.

Publications

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2. “Crystallization and preliminary X-ray diffraction analysis of human seminal plasma protein PSP94", M. Kumar, D. D. Jagtap, S. D. Mahale, V. Prashar, A. Kumar, A. Das, S. C. Bihani, J. L. Ferrer, M. V. Hosur and M. Ramanadhama, Acta Crystallographica Section F: Structural Biology and Crystallization Communications. (2009), 65, 389-391.
3. “Crystal Structure of Prostate Secretory Protein PSP94 Shows an Edge-to-Edge Association of two Monomers to Form a Homodimer", A. Kumar, D. Jagtap, S. D. Mahale, M. Kumar, Journal of Molecular Biology. (2010), 397, 947-956.
4. “Crystallization and preliminary X-ray diffraction analysis of Xaa-Pro dipeptidase from *Xanthomonas campestris*", A. Kumar, V. N. Are, B. Ghosh, U. Agrawal, S. N. Jamdar, R. D. Makde and S. M. Sharma, Acta Crystallographica Section F: Structural Biology and Crystallization Communications. (2014),70, 1268-71.

Technical Report:

1. “Conceptual Design Report for the High-Throughput Macromolecular Crystallography Beamline at the Indus-2", By A. kumar and Jagannath, BARC (External) Report (2007)

76. Name : **Pooja Saxena**
Enrolment No. : ENGG01201004001
Date of Award of degree : 03.08.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Design And Implementation Of Cmos Time-To-Digital Converter Asic For Ino Experiment.

Abstract

This thesis starts with the literature survey of various existing time interval lmeasurement techniques along with their merits and limitations, which paved away to design innovative TDCs with specifications provided by INO group. In the first endeavor, a low power 4-channel Vernier TDC ASIC with SPI based readoutand in-built digital calibrator is designed and fabricated using AMS 0.35 _mCMOS technology. The developed ASIC is functionally characterized and the achievedresolution (LSB) is 127 ps over 1.4 _s range. It is demonstrated to be a low power (43 mW @ 3.3V) as compared to earlier reported one (150 mW) in the same technology.This ASIC was subsequently interfaced with RPC detector FE electronics providing timing resolution (_ 2.6 ns) similar to that of commercial HPTDC. The Vernier TDC ASIC design is further enhanced with multi-hit capability and incorporation of four operating modes (time interval,common start, common stop and calibration) to achieve its utilization in INO experiment for multi-hit requirements as well as in other HEP experiments. It is carried out by conceptualizing a novel architecture of Vernier multi-hit TDC and successfully analyzing thescope of Vernier technique in negative time interval measurement. This 8-channel multi-hit Vernier TDC ASIC is designed for resolution of 100 ps over user selectable dynamic range one from 10 _s/20_s/30_s/60 _s. It can measure the minimum pulse width _ 1 ns of multi-hit signal. Moreover, for high event rate HEP experiments, a Flash technique based multi-hit TDC using a novel current balanced logic (CBL) delay element with the aim of improved resolution (<200 ps) in 0.35_m CMOS technology is designed.This four channel TDC is designed in time interval and common stop mode for resolution 150 ps over selectable dynamic range of 10 _s to 40 _s in steps of 10 _s and multi-hit pulse width measurement of _ 1 ns. The impact of PVT variations over the resolution is circumvented with the help of CBL delay element based delaylock loop. The scope of multi-hit Vernier and Flash TDC ASIC designs in this thesis is limited to their performance validation with the help of simulation results. The work carried out is discussed in eight chapters.

Publications

Journal

1. K. Hari Prasad, Menka Sukhwani, Pooja Saxena, V. B. Chandratre, ‘A Four Channel Time-to-digital Converter ASIC within-built Calibration and SPI Interface’, Nuclear Instruments and Methods in Physics Research A, vol. 737, pp.117-121, 2014.
2. Pooja Saxena, Sudheer K. M, V. B. Chandratre, ‘Design of Novel Current balanced Voltage controlled delay element’, International Journal of VLSI design & Communication Systems (VLSICS) vol.5, no.3, June 2014.
3. Pooja Saxena, K. Hari Prasad, V. B. Chandratre, ‘A Current Balanced Logic buffer based Time-to-Digital Converter with improved resolution’, Global Journal of Researches in Engineering: F Electrical and Electronics Engineering vol. 15 issue 4, 2015.
4. Pooja Saxena,K. Hari Prasad, V. B. Chandratre, ‘*Design of Multi-hit TDC using CBL delay element*’, International Journal of Electronics and Electrical Engineering, vol.5, no.1, July 2016 (under Print).

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1. Pooja Saxena, K. Hari Prasad, V. B. Chandratre, '*Comparative Analysis of tapped delay line architectures used in time stamping*', 60th DAE-BRNS National Symposium on Nuclear Physics, December 7-11, 2015, Sri Sathya Sai Institute of higher learning, Prasanti Nilayam.
2. Pooja Saxena, K. Hari Prasad, V. B. Chandratre, '*Implementation of Multi-hit Time-to-Digital Converter using Tapped Delay Line*', DAE-BRNS National Symposium on Nuclear Instrumentation, November 19-21, 2013, Training school- BARC, Anushakti Nagar, Mumbai.
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4. K. Hari Prasad, V. B. Chandratre, Pooja Saxena, C. K. Pithawa,'*FPGA based Time-to-Digital Converter*', Proceedings of DAE symposium on Nuclear Physics, vol.56, December 26-30, 2011, Andhra University, Visakhapatham.
5. Bheesette Satyanarayana, Sudeshna Dasgupta, Sonal Dhuldhaj, Naba Mondal, Nagaraj Panyam, Shobha Rao, Deepak Samuel, Mandar Saraf, Ravindra Shinde, Suresh Upadhya,Vinay Chandratre, Veena Salodia, Pooja Saxena, Menka Tewani, Satyajit Saha, Yogendra Viyogi, '*Electronics and data acquisition systems for RPC based INO ICAL detector', proceedings of XI Workshop on Resistive Plate Chambers and Related Detectors, POS (RPC2012)*,' February 5-10, 2012, laboratori Nazionali di Frascati,Italy.

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77. Name : **Radhakanta Dash**
Enrolment No. : ENGG01201104002
Date of Award of degree : 11.08.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Study Of Beam Dynamics In 100 Mev, 100 Kw Rf Electron Linac.

Abstract

Direct experimental studies of behaviour of the electron beam inside accelerator cavity are very difficult. Numerical simulations are, therefore powerful tools in the analysis of beam dynamics of present linear accelerator facilities as well as the future accelerators. This research work focuses on the beam dynamics of linear accelerator by analytical methods and computer simulations in order to predict the behavior and quality of the electron beam and minimize the beam loss. In this work, we have studied the beam dynamics of a 30 MeV standing wave, biperiodic, coupled cavity rf electron linac with the help of CST Microwave studio and ASTRA code to determine the optimized parameters for a nominal gain of energy of 30 MeV with minimum energy spread and keep the minimal growth of transverse emittance. This facilitates a safety operation of the linac and avoids induced radioactivity with hands on maintenance of the accelerating structure and components. Further we have studied the beam dynamics of a 10 MeV rf electron linac in operation and validate our simulation results with the experimental data within the limit of experimental errors. We present the beam dynamics results of a 100 MeV, 100 kW standing wave rf electron linac with the help of CST MWS, ASTRA and ELEGANT beam dynamics codes along with bunch compression scheme with chicken magnet that comprises four dipoles and compare the results with a 100 MeV traveling wave rf electron linac structure. We have presented analytical expressions for the growth of transverse emittance in an RF gap which includes the coupling between the phase spread of the beam and spherical aberration. Using reduced envelope equation for a laminar beam the shift in frequency of oscillation of the beam envelope in the RF field is calculated. Also, Analytical expression is derived for beam optics in a solenoid field considering terms up to the third order in the radial displacement. Two important phenomena: effect of

spherical aberrations in axial -symmetric focusing lens and influence of nonlinear space charge forces on beam emittance growth are discussed for different beam distributions. Chromatic aberration induced growth of emittance and distortion of phase space area is discussed. We have presented a new formulation for the aperture coupling problem in terms of Carlson Symmetric Integrals. The significance of such a method is that it considers the thickness of the aperture in to account to find the coupling coefficients between cavities unlike the earlier works which neglect the thickness of the aperture in aperture coupling problems. We have validated our theoretical model with the earlier works of aperture coupling taking thickness of the aperture tends to zero.

Publications

Journal

1. “Beam dynamics studies and parametric characterization of a standing wave electron linac”, R Dash, J Mondal, A Sharma and K C Mittal, *Journal of Instrumentation,* 2013, *8 T07002*, 1-19.
2. “Numerical evaluation of aperture coupling in resonant cavities and frequency perturbation analysis”, R Dash, B Nayak, A Sharma and K C Mittal, *Journal of Instrumentation*, 2014, *9 P01012*, 1-14.
3. “Effect of Spherical Aberration on the Emittance Growth and frequency of Oscillation of a Beam Crossing an RF Gap”, B Nayak, R Dash and K C Mittal, *Nucl. Instr. and Meth. A*, 2014, *746*, 1-3.
4. “Analysis of Transverse RMS Emittance Growth of a Beam induced by Spherical and Chromatic Aberration in a Solenoidal Field”, R Dash, B Nayak, A Sharma and K C Mittal, *Nucl. Instr. and Meth. A*, 2016, *807*, 94-100.

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2. “Study of Beam Dynamics of a 30 MeV Standing Wave Electron Linac”, R Dash, J Mondal, A Sharma and K C Mittal, INPAC-2013, Kolkata, November 2013.
3. “Beam dynamics studies of a 10 MeV standing wave electron linac”, R Dash, A Sharma and K C Mittal, 26th International Symposium on Discharges and Electrical Insulation in Vacuum,ISDEIV-2014,Mumbai, September 2014.
4. “Numerical evaluation of aperture coupling in resonant waveguides and frequency perturbation analysis”, R Dash, B Nayak, A Sharma and K C Mittal, 26th International Symposium on Discharges and Electrical Insulation in Vacuum 2014,ISDEIV-2014, Mumbai, September 2014.
5. “Study of beam dynamics of a 100 MeV electron linac”, R Dash, B Nayak, A Sharma and K C Mittal, 26th International Symposium on Discharges and Electrical Insulation in Vacuum 2014,ISDEIV-2014, Mumbai, September 2014.
6. “Beam dynamics simulation studies of a 30 MeV electron linac”, R Dash, B Nayak, A Sharma and K C Mittal, National Symposium on Vacuum Technology & Its Applications to Electron Beams, IVSNS-2015, Mumbai, November 2015.
7. “Beam dynamics study of a 100 MeV RF electron linac”, R Dash, B Nayak, A Sharma and K C Mittal, International Conference on Microwave, Optical and Communication Engineering, ICMOCE-2015, Bhubaneswar, December 2015.

78. Name : **Tushar Debnath**
Enrolment No. : CHEM01201104033
Date of Award of degree : 17.08.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Ultrafast Charge Transfer Dynamics In Solar Cell Materials.

Abstract

The present thesis summarizes the synthesis and characterization of different nanostructured materials through X-ray diffraction spectroscopy, transmission electron microscopy and optical spectroscopy (UV-Vis absorption and photoluminescence). Charge transfer and exciton dynamics involving different nanostructured materials have been investigated with the aid of femtosecond transient absorption and nanosecond time resolved emission spectroscopy. Interfacial electron transfer dynamics of two newly synthesized structurally similar coumarin dyes (C1 and C2) on TiO2 nanoparticles have been demonstrated where C1 exist as intramolecular charge transfer (ICT) state in polar solvent, C2 exist as both ICT and twisted intramolecular charge transfer (TICT) state. Involvement of TICT states in C2 in C2/TiO2 system is the reason for higher electron injection yield and also slower back electron transfer. However formation of TICT state becomes restricted on Au NP surface due to restricted molecular rotation of diethyl amino group as observed of C3 molecule. Ultrafast electron and hole transfer dynamics have been demonstrated in CdSe quantum dot (QD), CdSe/ZnS Type-I core-shell and CdSe/CdTe Type-II core-shell after sensitizing the QD materials by aurin tricarboxylic acid (ATC), where CdSe QD and ATC form charge transfer (CT) complex. Essential conclusion was hole transfer process is most efficient in CdSe QD, on the other hand it has been facilitated in CdSe/CdTe type II and retarded in CdSe/ZnS type I coreshell materials. Effect of molecular coupling in two Re(I)−polypyridyl complexes having pendent catechol (Re1,2) and resorcinol (Re1,3) as the coupling element on CdSe QD surface has been studied where charge recombination was found to be slower in Re1,3/CdSe system as compared to that of Re1,2/CdSe system due to weaker electronic coupling in the former system. Similar result was obtained in wide band gap ZnS-tri phenyl phenyl methane (TPM) composite where TPM dye having weak coupling (e.g. ATC, weak carboxylic coupling vs. PGR, strong catechol coupling) has slower charge recombination. In addition it is also demonstrated by incorporating electron donating and withdrawing moiety in phenol, tuning of hole and electron transfer process from photoexcited CdSe QD to phenols. Specially aligned surface accumulated Mn doped NCs were explored to study the effect of dopant atom on charge carrier dynamics in NC materials. Strong CT complex followed by extremely slower charge recombination was found in Mn doped CdSe NC sensitized BrPGR molecule than the undoped case which signifies Mn centre as electron storage centre. The effect of Mn atom on the charge transfer state of alloyed CdTeSe nanocrystals has been preciously described, which showed unusually slow electron cooling (~700ps) from Mn 3d state to charge transfer state and slower recombination. An unprecedented increment of 3.3% to 4.29% of photocurrent conversion efficiency (PCE) was observed in Mn doped CdZnSSe gradient alloy when compared to the undoped case. A comparison of homogeneous and gradient CdZnSSe alloy has been proposed in the light of higher solar conversion efficiency (4.5%) in the former. A detailed spectroscopic investigation of $CuInS_2$ (CIS) NCs in the relevance of sub-picosecond exciton and bi-exciton dynamics also has been unraveled.

Publications

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2. “Super Sensitization: Grand Charge (Hole/Electron) Separation in Aurin Tricarboxylic Acid (ATC) dye Sensitized CdSe Quantum Dot, CdSe/ZnS Type-I and CdSe/CdTe Type-II Core-shell Quantum Dot Materials” Tushar Debnath, Partha Maity and Hirendra N. Ghosh. Chem. Eur. J 2014, 20, 13305-13313.
3. “Electron Trap to Electron Storage Centre in Specially Aligned Mn doped CdSe d-Dot: A Step forward on the Design of Higher Efficient Quantum Dot Solar Cell” Tushar Debnath, Partha Maity, Sourav Maiti and Hirendra N. Ghosh. J. Phys. Chem. Lett. 2014, 5, 2836−2842.
4. “Restriction of Molecular Twisting on Au nanoparticle Surface” Tushar Debnath, Partha Maity, Jayanta Dana, Hyacintha Lobo, Ganapati S. Shankarling, and Hirendra N. Ghosh. Chem. Eur. J 2015, 21, 5704 – 5708.
5. “Ultrafast Electron Injection, Hole Transfer and Charge Recombination Dynamics in CdSe QD Super-Sensitized Re(I)−Polypyridyl Complexes with Catechol and Resorcinol moiety: Effect of Coupling” Tushar Debnath, Partha Maity, Tanmay Banerjee, Amitava Das, and Hirendra N. Ghosh. J. Phys. Chem. C 2015, 119, 3522-3529.
6. “Subpicosecond Exciton Dynamics and Biexcitonic Feature in Colloidal $CuInS_2$ Nanocrystals: Role of In–Cu Antisite Defects” Tushar Debnath, Sourav Maiti, Partha Maity and Hirendra N. Ghosh. J. Phys. Chem. Lett. 2015, 6, 3458-3465.
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8. “Unusually Slow Electron Cooling to Charge Transfer State in Gradient CdTeSe Alloy Nanocrystal Mediated Through Mn Atom” Tushar Debnath, Sourav Maiti and Hirendra N. Ghosh. J. Phys. Chem. Lett. 2016 7, 1359–1367.
9. “Tuning Hole and Electron Transfer from Photo-excited CdSe Quantum Dot to Phenol Derivatives: Effect of Electron Donating and Withdrawing Moiety” Tushar Debnath, Deepa Sebastian, Sourav Maiti and Hirendra N. Ghosh. J. Phys. Chem. C 2016, (Communicated).
10. “An Insight of Molecular Twisting on Semiconductor and Metal Nanoparticle Surface” Tushar Debnath and Hirendra N. Ghosh. J. Photochem. Photobiology. C: Review 2016, (To be communicated).
11. “Promising Enhancement of Power Conversion Efficiency of Homogeneous Alloy than Gradient Alloy and the Role of Mn as Electron Storage Centre: An Insight of Interface through Excited State Dynamics” Tushar Debnath, Kausturi Parui, Sourav Maiti and Hirendra N. Ghosh. (To be communicated)

79. Name : **Sayali Kulkarni**
Enrolment No. : LIFE01201204001
Date of Award of degree : 17.08.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Bioremediation of uranium from acidic and alkaline solutions using genetically engineered Deinococcus radiodurans

Abstract

The thesis embodies work aimed at genetically engineering a highly radioresistant microbe, *Deinococcus radiodurans*, to bioprecipitate uranium from alkaline radioactive waste solutions, to extend its working to a broad pH range and optimising the remediation protocols. Towards this goal, a non-specific acid phosphatase (PhoN) from *Salmonella typhimurium* and a high specific activity novel alkaline phosphatase (PhoK) from *Sphingomonas* sp. strain BSAR-1, were cloned and mobilised in to *E. coli* and *D. radiodurans* by designing appropriate recombinant DNA technology to construct strains *Deino-PhoN* and *Deino-PhoK, respectively*. Pyramiding of both the *phoN* and *phoK* genes in a single *D. radiodurans* strain (*Deino-PhoNK*) was also accomplished successfully.

Expression of the phosphatase genes, driven from a strong Deinococcal promoter P_{groESL} resulted in high level expression and activity of both phosphatases - the PhoN in the periplasmic space and PhoK in periplasm but also released extracellularly, in the recombinant strains. All three strains also achieved efficient precipitation of U as uranyl phosphate even after exposure to 6 kGy of ^{60}Co γ-rays. The *Deino-PhoK* strain was far more active in U precipitation than the *Deino-PhoN* strain at any pH, while *Deino-PhoNK* strain exhibited activities comparable to *Deino-PhoN* (pH 6.8) or *Deino-PhoK* (pH 9.0) strains at their respective pH optima. XRD analyses identified precipitate under both pH conditions to be identical as chernikovite or meta-autunite, which showed strong green fluorescence upon exposure to UV providing a handy tool for monitoring U precipitation. Elegantly designed transmission electron microscopy based experiments established that the location of the precipitated U (cell-bound or extracellular) was determined by aqueous uranium speciation and not by the location of the enzyme. Lyophilisation achieved excellent preservation of cells (and the enzyme activity contained therein) for >2 years at ambient temperatures, thus achieving volume reduction and extension of shelf life. Such cells also accomplished U precipitation over a wide range of U concentrations to result in very high loading of up to 10g U/g biomass under alkaline conditions. The extracellularly precipitated uranyl phosphate under alkaline conditions could be immobilised in alginate beads to facilitate containment and easy recovery of this toxic metal. Immobilised recombinant cells as well as purified PhoK enzyme efficiently precipitated U in a column based flow-through system, though batch process turned out to be more efficient due to (a) clogging of column by the precipitate, and (b) poisoning of enzyme by prolonged exposure to uranium at room temperature.

Publications

Journal

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2. Sayali Kulkarni, Chitra Seetharam Misra, Alka Gupta, Anand Ballal and Shree Kumar Apte* Interaction of uranium with bacterial cell surface: Implications from phosphatase mediated uranium precipitation- (Appl. Env. Microbiol. doi:10.1128/AEM.00728-16).

Conference

1. Kulkarni S, Misra C, Ballal A, Gupta A, Apte S.K. (2014) Studies on phosphatase mediated bioprecipitation in recombinant *E. coli* / *D. radiodurans* using electron microscopy;

International Conference on Electron Microscopy and XXXV Annual Meeting of Electron Microscopy Society of India (EMSI-2014); Page 205 (P-IC318); University of Delhi, Delhi, India.

2. Kulkarni S, Misra C, Gupta A, Ballal A, Apte S.K. (2015) Effect of pH /uranyl species on localization of uranyl phosphate precipitate in recombinant *D. radiodurans* expressing PhoN/PhoK; DAE-BRNS Life Science Symposium, 2015, page- 142 (P-50), Mumbai, India.
3. Ballal A, Kulkarni S, Misra C, Gupta A, Apte S. K. (2015) Transmission electron microscopy to visualize the localization of uranyl phosphate precipitate in *E. coli ;* Conference on Electron Microscopy and XXXVI Annual Meeting of Electron Microscopy Society of India (EMSI-2015); Page 301; CIDCO convention centre, Vashi, Navi Mumbai.

* * *

80. Name : **Archana Mishra**
Enrolment No. : PHYS10200904008
Date of Award of degree : 22.08.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Study Of Interactions In The Hofstadter Regime Of The Honeycomb Lattice.

Abstract

The recent realization of Hofstadter butterfly in moire superlattices and realization of the Hofstadter Hamiltonian in the square lattice in cold atom systems has motivated me to study the effect of interactions in the Hofstadter regime of the honeycomb lattice. My main aim in this work is to understand the interaction induced complex phases in detail and study the topology and geometry of the ground state of the system. Interactions induces charge ordering which break the translational and rotational symmetry of the system giving rise to anisotropic phases as the ground state for this system. The anisotropy in the particle density can be characterized by quadrupole and dipole moments and the phases are accordingly classified to symmetric phase, charge density wave, nematic phase and ferrielectric phase. Some of these Landau phase transitions are accompanied with the change in the topology of the system thus giving examples of topological transitions from non-zero Hall conductivity phase to zero Hall conductivity phase. I try and give an insight to these topological transitions. Throughout the range of interaction strength considered, the energy gap never closes and hence the mean field approximation is an good approximation here. Further, I also study the geometry of the ground states and investigate the structure of the anisotropic phases by studying pair correlations from the point of view of the quantum geometric approach to insulating states. I extended the above framework to include the magnetic flux per plaquette of the form p/q where p,q are coprime integers and $p < q$. I consider $q \in [3, 20]$ and solve the interacting Hamiltonian using mean field theory for filled band cases and main aim of this work is to study the effect of interactions on the Hofstadter butterfly. By studying the energy flux diagram and the Landau fan diagram, I see that the fractal structure in the Hofstadter butterfly gets more and more disintegrated with the increase in the interaction strength. As the interaction strength increases, the number of phase transitions to translational symmetry breaking phases increases. This breaking of translational symmetry introduces a new length scale in the system which leads to the disintegration of the fractal nature of the energy flux diagram. Many of these phase transitions are accompanied with the change in the Hall conductivity of the system. These topological transitions also increase with the increase in the interaction strength and hence, the disintegration of the Hofstadter butterfly gets manifested in the Landau fan diagram. I also propose a method to probe the Berry curvature in the optical lattice system. The confining trap breaks particle-hole symmetry and makes the Berry curvatures of the bands observable. I have shown that the effect of this is seen in the rotation of the expanding cloud when the trap is removed. For realistic atomic and trap parameters, I have shown that this provides a clear signal in time-of-flight experiments.

Publications

Journal

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2. Archana Mishra, S. R. Hassan, R. Shankar, “Effects of interaction in the Hofstadter regime of the honeycomb lattice”, Phys. Rev. B 93, 125134 (2016).
3. Archana Mishra, S. R. Hassan, R. Shankar, “Translational symmetry breaking and the disintegration of the Hofstadter butterfly”, arXiv:1605.06307 (Submitted to Physical Review B)

* * *

81. Name : **K.V. Vivekananda**
Enrolment No. : CHEM01200904015
Date of Award of degree : 22.08.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Synthesis And Characterization Of Multinuclear/ Supra-Molecular Complexes Of Platinum Group Metals With Chalcogen Ligands.

Abstract

The main focus of this thesis is based on coordination/transition metal (Pt/Pd) driven self-assemblies with chalcogen ligands which represent a powerful synthetic methodology for multi-nuclear systems with well-defined architectures. In this regard, the non-chelating bidentate ligands such as 4-pyridyl chalcogenolate, 3-/4-mercaptobenzoic acids and aryldithiol ligands have been employed in the design of Supramolecular assemblies. In the first section 4-pyridyl selenolate complexes of Pd(II)/Pt(II) have been studied. These ligands offer several bonding possibilities with a metal ion unlike in the case of chelating 2-pyridyl chalcogenolate ligand. Catalytic activity of some of the palladium complexes has been explored. In the second section supramolecular assemblies of Pd(II)/Pt(II) were synthesized by employing 3-/4-meracptobenzoic acid ligands. These complexes stabilize themselves through hydrogen bonding in solid state. In the third section simple and readily available aryldithiol ligands were used in the construction of Pd(II)/Pt(II) macrocycles which are stable in the solid state as well as in solution. These macrocyclic complexes showed excellent catalytic activity in Suzuki-Miyaura reactions with high turn-over numbers. In the fourth section 4-pyridyl tellurolate complexes of Pd(II)/Pt(II) were synthesized which showed distinct reactivity from analogous 2-pyridyl derivatives giving some serendipitous formation of products by cleavage and new formation of Te–C bonds. In the last section chemistry of macrocyclic Pt/Pd complexes of 4,4'-dipyridylditelluride/diselenide ligand formed *via* self-assembly were reported. Binuclear complexes having different bridging atoms with metal centers were confirmed by X-ray diffraction analysis. The thesis led to several international journals and conferences.

Publications

Journal

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coupling reactionK. V. Vivekananda, S. Dey, A. Wadawale, N. Bhuvanesh and V. K. Jain*Dalton Trans.*, 42 (2013) 14158-14167.

2. Supramolecular 3-/4-mercaptobenzoic acid complexes of palladium(II) and(II) stabilized by hydrogen bondingK. V. Vivekananda, S. Dey, A. Wadawale, N. Bhuvanesh, and V. K. Jain*Eur. J. Inorg. Chem.*, (2014) 2153-2161.
3. Supramolecular macrocyclic Pd(II) and Pt(II) squares and rectangles with aryldithiolate ligands and their unprecedented catalytic activity in Suzuki C−C coupling reactionK. V. Vivekananda, S. Dey, D. K. Maity, N. Bhuvanesh and V. K. Jain *Inorg. Chem.*, 54 (2015) 10153-10162.
4. Molecular architecture and self assembly of hemilabile organoselenium/ telluriumcomplexes of palladium and platinumK. V. Vivekananda, S. Dey, N. Bhuvanesh and V. K. Jain (manuscript to be submitted in EurJIC)
5. Synthesis and characterization of unprecedented formation of Pt/Pd complexes with 4-pyridyltellurolate ligandK. V. Vivekananda, S. Dey, A. Wadawale, N. Bhuvanesh, V. K. Jain (manuscript to be submitted).
6. Silver(I) coordination polymer of 4,4'-dipyridyl selenide and its solvothermolysisGoutam Kumar Kole, K. V. Vivekananda, Mukesh Kumar, S. Dey and V. K. Jain*International Journal of Chemistry*, 3 (3) (2014) 263-268.
7. Hemilabile silver(I) complexes containing pyridyl chalcogenolate (S, Se) ligands and their utility as molecular precursors for silver chalcogenidesGoutam Kumar Kole, K. V. Vivekananda, Mukesh Kumar, Rakesh Ganguly, S. Dey and V. K. Jain*CrystEngComm*, 17 (2015) 4367-4376.

Conferences

1. “Syntheses of Pt(II) complexes with non-chelating 4-pyridylselenolate ligand ranging from mononuclear to supramolecular structures”K. V. Vivekananda, S. Dey, V. K. Jain and N. Bhuvanesh4th DAE-BRNS Interdisciplinary Symposium on Materials Chemistry during 11th - 15th December 2012, held at Bhabha Atomic Research Centre, Mumbai.
2. “Palladium (II) and platinum (II) complexes with 4-pyridylselenolate ligand”K. V. Vivekananda, S. Dey, V. K. Jain and N. Bhuvanesh“7th CRSI-RSC Symposium in Chemistry and 15th CRSI National Symposium inChemistry” during January 31st - February 3rd 2013, held at Banaras Hindu University, Varanasi.
3. “Supramolecular assemblies of palladium(II) and platinum(II) complexes with 3-/4-mercaptobenzoic acid via hydrogen bonding” K. V. Vivekananda, S. Dey, A. Wadawale, N. Bhuvanesh and V. K. Jain“5th DAE-BRNS Interdisciplinary Symposium on Materials Chemistry” during 9th - 13th December 2014, held at Bhabha Atomic Research Centre, Mumbai.
4. Participated in “3rd DAE-BRNS Interdisciplinary Symposium on Materials Chemistry” during December 2010, held at Bhabha Atomic Research Centre, Mumbai.

82. Name : **Partha Maity**
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Constituent Institute : Bhabha Atomic Research Centre,
Title : Ultrafast Charge Transfer Dynamics In Quantum Dots And Quantum Dots/Molecular Adsorbate

Abstract

The main emphasis of this thesis is ultrafast charge transfer dynamics of the nanocrystals quantum dots in absence and in presence of molecular adsorbate. The charge transfer dynamics have been demonstrated using different NCs in terms of colloidal quantum dots, core/shell, alloys and the various organic and inorganic molecules. The NCs have been synthesized in non aqueous medium and the morphology are analyzed by XRD, HRTEM, EDX, and optical techniques. The charge carrier dynamics of the composite system have been carried out using time resolved PL and femtosecond transient absorption study. The NCs in different form are employed gradually depending on their application in QDSC. To improve photo-current conversion efficiency in QDSC, the molecular adsorbates have been introduced with the NCs which develop charge separation and prevent the exciton annihilation. This thesis has nine different chapters including general introduction of quantum dots nanocrystals, experimental setups, and summary and outlooks. The experimental conclusions are relevant towards QDSC are discussed in chapter three to eight. Chapter 3 describes the charge transfer interaction of CdS QD in presence of 4 ,5 -dibromo fluorescence and two BODIPY (borondipyrro methene derivative) dyes. Limited absorption cross-section and strong exciton annihilation of the CdS QDs have been optimized by introducing DBF and the BODIPY molecules respectively. Different charge transfer processes in colloidal perovskite $CsPbBr_3$ QDs in presence of DBF molecule are described in chapter 4. Quenching of the CPB QDs luminescence with selective photo-excitation reveals photo-excited hole transfer from CPB QD to DBF molecule. Work presented in chapter 5 is band gap engineering and controlling charge carrier delocalization in two different core/shell NCs, CdS/CdSe inverted type I and CdSe/CdS quasi type II, utilizing femtosecond transient absorption spectroscopy in absence and presence of different quencher molecule (electron quencher BQ and hole quencher Py). The structural properties of the NCs has been analyzed with the help of quenching study. Ultrafast hole- and electron-transfer dynamics in different core/shell (CdS/CdSe and CdS/CdTe) NCs sensitized by different molecular adsorbates are demonstrated in chapter 6. Chapter 7 describes carrier cooling dynamics of CdS_xSe_{1-x} and $Cd_xZn_{1-x}Se$ alloy QD. Chapter 8 deals composition controlled size quantization of CdS_xSe_{1-x} alloy QD for developing third generation QD solar cell. Varying the composition of the constituent, it has been observed that CdS_xSe_{1-x} alloy QDs is the superior sensitizer as compare to both CdS as well as CdSe.

Publications

Journal

1. "Ultrafast Hole and Electron Transfer Dynamics in CdS/Di-bromofluorescein (DBF) Super-Sensitized Quantum Dot Solar Cell Materials", Partha Maity, Tushar Debnath and Hirendra N. Ghosh, *J. Phys. Chem. Lett.,* 2013, *4*, 4020–4025.*
2. "Cascading Electron and Hole Transfer Dynamics in CdS/CdTe Core-Shell Sensitized Bromo-Pyrogallol Red (Br-PGR): Slow Charge Recombination in Type II Regime", Partha Maity, Tushar Debnath, Uday Chopra, Hirendra N. Ghosh, *Nanoscale,* 2015, *7*, 2698-2707.*
3. "Slow Electron Cooling Dynamics Mediated by Electron-Hole Decoupling in Highly Luminescent CdS_xSe_{1-x} Alloy Quantum Dots", Partha Maity, Tushar Debnath and Hirendra N. Ghosh, *J. Phys. Chem. C,* 2015, *119*, 10785−10792.*
4. "Ultrafast Charge Carrier Delocalization in CdSe/CdS Quasi-Type II and CdS/CdSe Inverted Type I Core–Shell: A Structural Analysis through Carrier-Quenching Study", Partha Maity, Tushar Debnath and Hirendra N. Ghosh, *J. Phys. Chem. C*, 2015, *119*, 26202-26211.*

5. "Slow Electron Cooling Dynamics of Highly Luminescent CdS_xSe_{1-x} Alloy Quantum Dot", Partha Maity, Tushar Debnath and Hirendra N. Ghosh, *Ultrafast Phenomena XIX*, 2014, Springer Proceedings in Physics 162 (pp-275-278), DOI 10.1007/978-3-319-13242-6_67.*
6. "Charge De-localization in the Cascade Band Structure CdS/CdSe and CdS/CdTe Core-Shell Sensitized with Re (I)−polypyridyl Complex", Partha Maity, Tushar Debnath, Tanmay Banerjee Amitava Das, and Hirendra. N. Ghosh, *J. Phys. Chem. C,* 2016, 120, 10051-10061.*
7. "Ultrafast Charge Transfer Dynamics in Totally Inorganic Colloidal $CsPbBr_3$ Perovskite Quantum Dots Sensitized by 4,5-di bromo fluorescence" Partha Maity, Jayanta Dana and Hirendra Nath Ghosh, (Accepted in Ultrafast Phenomena 2016).*
8. "Multiple Charge Transfer Dynamics in Colloidal $CsPbBr_3$ Perovskite Quantum Dots Sensitized Molecular Adsorbate", Partha Maity, Jayanta Dana and Hirendra Nath Ghosh, *J. Phys. Chem. C,* 2016, 120 (Accepted)*
9. "Improving the Solar Cell Efficiency Utilizing CdSSe Alloy Quantum Dots" Partha Maity, Sourav Maiti, Tushar Debnath, Sourav K. Guin, Jayanta Dana and Hirendra Nath Ghosh, *J. Phys. Chem. C,* 2016 Submitted.*
10. "Hole Delocalization Develops Exciton Population and Extend of Charge Separation in Highly Luminescent CdSe rich $Cd_xZn_{1-x}Se$ Gradient Alloy QD" Partha Maity, Jayanta Dana and Hirendra Nath Ghosh, *J. Phys. Chem. C,* 2016 Submitted.*
11. "Sensitization of BODIPY Molecule through Förster Resonance Energy Transfer from Photo-excited CdS Quantum Dot" Partha Maity, Tushar Debnath, Thumuganti Gayathri, Surya Prakash Singh, and Hirendra N. Ghosh, *Chemistry-A European Journal* (Submitted).*

Conferences:

1. "Cascading Electron and Hole Transfer Dynamics in CdS/CdTe Core-Shell Sensitized Bromo-Pyrogallol Red (Br-PGR): Slow Charge Recombination in Type II Regime", Partha Maity, Tushar Debnath, Uday Chopra, Hirendra N. Ghosh, *Trombay Symposium on Radiation & Photochemistry (TSRP-2014),* BARC, Mumbai, India.*
2. "Charge De-localization in the Cascade Band Structure CdS/CdSe and CdS/CdTe Core-Shell Sensitized with Re (I)−polypyridyl Complex", Partha Maity, Tushar Debnath, Tanmay Banerjee Amitava Das, and Hirendra. N. Ghosh, *16th CRSI National Symposium in Chemistry (CRSI-2014),* IIT Bombay, India.*
3. "Ultrafast Hole and Electron Transfer Dynamics in CdS/Di-bromofluorescein (DBF) Super-Sensitized Quantum Dot Solar Cell Materials", Partha Maity, Tushar Debnath and Hirendra N. Ghosh, *Sixth International Conference on Nano Science and Technology (ICONSAT-2014),* INST Chandigarh, India.*
4. "Slow Electron Cooling Dynamics of Highly Luminescent CdS_xSe_{1-x} Alloy Quantum Dot", Partha Maity, Tushar Debnath and Hirendra N. Ghosh, *19th International Conferences on Ultrafast Phenomena (UP-2014),* Okinawa, Japan.*
5. "Sensitization of BODIPY Molecule through Förster Resonance Energy Transfer from Photo-excited CdS Quantum Dot" Partha Maity, Tushar Debnath, Thumuganti Gayathri, Surya Prakash Singh, and Hirendra N. Ghosh, *Interdisciplinary Symposium for Materials Chemistry (ISMC-2014),* BARC, Mumbai, India.*
6. "Hole Delocalization Develops Exciton Population and Extend of Charge Separation in Highly Luminescent CdSe rich $Cd_xZn_{1-x}Se$ Gradient Alloy QD" Partha Maity, Jayanta Dana and Hirendra Nath Ghosh, *Frontiers in Advanced Materials (FAM-2015)*, IISC, Bangalore, India.*
7. "Ultrafast Charge Carrier Delocalization in CdSe/CdS Quasi-Type II and CdS/CdSe Inverted Type I Core–Shell: A Structural Analysis through Carrier-Quenching Study", Partha Maity, Tushar Debnath and Hirendra N. Ghosh, *Trombay Symposium on Radiation & Photochemistry (TSRP-2016),* BARC, Mumbai, India.*

83. Name : **G. Veda Prakash**
Enrolment No. : ENGG06201104001
Date of Award of degree : 25.08.16
Constituent Institute : Institute For Plasma Research
Title : Compact Pulsed Power Systems Using Liquid Dielectrics.

Abstract

In the recent past, the demands for pulsed power machines have increasedto number of applications. Many suchapplications require compact and low weight pulsed power systems with high voltage output (>100 kV). The portability and compactness of pulsed power systems can be accomplish by using dielectric medium with high dielectric constant and good breakdown strength. In comparison with solid dielectrics, liquids and gases are self-healing. High dielectric constant and good breakdown strength make liquids more suitable for energy storage and as switch media compared to compressed gases, particularly for nanosecond pulse generators.Proper understanding of the breakdown properties of dielectrics will lead to improve the dielectric strength. Despite extensive research and theoretical studies, the understandings of electrical breakdown properties of liquids (like water) are far from complete. In this work, an effort has been made to understand the electrical breakdown properties of water under nano second regime with the help of Tesla based pulse generator.Further, in order to understand to estimate the electrical breakdown properties of liquids, fast response electrical diagnostics *viz.*, capacitive voltage sensor and self-integrating Rogowski coil are indigenously developed and calibrated using standard commercial probes. Experiments have been carried out by applying tens of nanosecond pulses and hundreds of kilo volts under uniform field conditions. The parametric effect like, effect of electrode material (Brass and Stainless steel)and change in distance between the electrodes on water breakdown propertieshave been studied. In addition, to understand the observed effect of electrode material (i.e. stainless steel and brass) is analyzed by using the optical emission spectra during the discharge. The spectra data confirms the presence of charge during discharge which suggests that the shielding effect at electrode surface reduces the electric field. The comparative study of electrical breakdown properties of deionized water (H_2O) and heavy water (D_2O) is presented with two different electrode materials (SS and Brass),and polarity (positive, negative) combinations.Further, to understand breakdown behavior it is attempted to know the change in chemical behavior in both liquids due to discharge by using optical Fourier transform infrared (FTIR) absorption spectroscopy. This enables a qualitative interpretation of the superior performance exhibited by H_2O as a dielectric for compact pulsed power applications. In order to understand the physical processes of discharge initiation in the pulsed breakdown of liquids and the basic laws of formation and propagation of discharges in liquid a high speed fast optical photo recording(Stanford computer optics, 4 Picos, ICCD) camera has been used.The breakdown images present the initiation and propagation of streamer from the electrode into the dielectric medium in the nanosecond regime.

Publications

Journal

1. Tesla based pulse generator for electrical breakdown study of liquid dielectrics, G.VedaPrakash, R.Kumar, J.Patel, K.Saurabh, and A.Shyam Rev. Sci. Instrum. 84, 126108 (2013), dx.doi.org/10.1063/1.4850529.
2. Comparative study of Electrical breakdown properties of Deionized Water and Heavy water under pulsed power conditions,G.VedaPrakash, R.Kumar, J.Patel, K.Saurabh, and AnithaV.P, M.B. Chowdari andA.Shyam,. Rev. Sci. Instrum. 87, 015115 (2016), dx.doi.org/10.1063/1.4940420
3. Study of anode initiated breakdown properties of water, G.VedaPrakash, R. Kumar, S. Kumar, A.Shyam, IEEE transactions on plasma science (Under Review-TPS9117R1).

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1. Electrical breakdown study of water under nanosecond pulsed conditions using optical diagnostic,G.VedaPrakash, Kumar, R. Kumar, S. A.Shyam, in *Pulsed Power Conference (PPC), 2015 IEEE* , pp.1-3, May 31 2015-June 4 2015, doi: 10.1109/PPC.2015.7296947

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84. Name : **Atanu Kumar**
Enrolment No. : ENGG05200904001
Date of Award of degree : 25.08.16
Constituent Institute : Saha Institute of Nuclear Physics,
Title : Evolution Of Cosmological Perturbation Through Bounce In Covariant Perturbations Theory And Tests Of Linearity.

Abstract

In spite of the success of standard cosmological model in providing a more or less accurate description of our Universe, it suffers from some inherent difficulties. Some of these difficulties were addressed by assuming an inflationary phase in the history of expansion of the Universe. However the initial singularity, which results in the breakdown of the classical description of spacetime, is not removed in inflationary models. Models of nonsingular universe, with a contracting phase followed by a bouncing phase and an expanding phase, has been studied for long. Recently it is observed that bouncing model with a dust dominated contracting phase can generate scale invariant spectrum of curvature perturbation. But in order to observe this spectrum in expanding phase, the perturbations are required to evolve smoothly through the bounce. Growth of perturbations in the contracting phase raised some doubts on the validity of linear perturbation theory around bounce and preservation of scale invariant spectrum. In the standard coordinate based perturbation theory, the perturbations ar observed to grow in some gauges, while they remain small in some other gauges. In this thesis I have suggested an alternative test of linearity using covariant perturbation theory. This test involves the investigation to find whether the nonlinear terms are truly small compared to the linear terms. For this purpose, some linearity parameters are defined as the ratio of nonlinear and linear terms. For dust and radiation dominated collapsing backgrounds, these parameters are found to diverge as the scale factor shrinks to zero.This formalism is applied to a simple and nonsingular bounce. The bounce is observed in a model having two components of perfect fluids---one is a normal fluid component with a dust-like equation of state and the other has a negative energy density and radiation-like equation of state. The fluid violates the null energy condition close to the bounce. Gauge invariant perturbations are defined in terms of the comoving observers. The tensor perturbations remain finite and well behaved at and close to the bounce but scalar and vector perturbations become singular at the turning point which is the boundary of the spacetime region where the null energy condition is violated. Besides the constant adiabatic mode, the comoving curvature perturbation has a non-adiabatic mode that diverges at the turning point. By computing the growth of linearity parameters it has been shown that the perturbations do not remain linear at the turning point. The matching conditions for scalar perturbations are also studied and the covariantly defined curvature perturbation is found to be the correct variable to be matched across transition surfaces to get correct spectrum.

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85. Name : **Rupa Mishra**
Enrolment No. : LIFE09200904003
Date of Award of degree : 29.08.16
Constituent Institute : Tata Memorial Centre
Title : Molecular Insights into p53 repressed anti-apoptotic proteins, Clusterin and Survivin in human oral cancer.

Abstract

Background: p53, a tumor suppressor protein is inactivated in approximately half of the oral cancer cases. Earlier studies from the lab show altered expression of the p53 targets clusterin and survivin in oral cancer cell lines and tissues. The current study thus aimed to identify the ability of the p53 family protein, p63 in regulating clusterin and survivin expression and its role in oral tumorigenesis. Methods: The transcript and protein expression of p63, clusterin and survivin was determined by qPCR and western blotting. The role of p63 in oral tumorigenesis was assessed by knockdown of p63 and its effects on invasion, migration and proliferative capacity of oral cancer cell lines with differing p53 background. Results: Our studies show an upregulation of all survivin isoforms in oral cancer cell lines and tissues as well as predominant expression of ΔNp63 and secretory clusterin. Our studies also demonstrate that mutant p53 is capable of binding to p63 in vitro and affects the functions of p63. p63 activates survivin expression in the presence of the R273H mutant p53 whereas in the absence of a functional p53, p63 represses survivin expression. Similarly the tumorigenic properties regulated by p63 were also found to be affected by the presence of mutant p53. p63 knockdown showed reduced migration in irrespective of the p53 status of the cell lines. However in the absence of a functional p53, p63 knockdown resulted in increased invasion whereas in the presence of a mutant p53 p63 knockdown resulted in decreased proliferative ability. Gene expression analysis identified genes involved in NOTCH signaling, Wnt Signaling and TGFβ signaling to be under the regulation of p63 in oral cancer cells.
Conclusion: Our studies thus demonstrate that p63 plays a role in oral tumorigenesis and also that the functions of p63 in oral cancer cells may be affected by the presence of the R273H mutant p53. This is the first study to show a gain of function role of the R273H mutant in oral cancers. Since oral cancers are frequently associated with mutations in p53, identification of the specific pathways activated by the mutant forms may provide a better approach to drug discovery and therapy.

Publications

Journal

1. High expression of survivin wt and its splice variants survivin ΔEx3 and survivin 2B in oral cancers. Rupa Mishra, Vinayak Palve, Sadhana Kannan, Sagar Pawar and Tanuja Teni Oral Surg Oral Med Oral Pathol Oral Radiol, 2015, DOI: 10.1016/j.oooo.2015.06.027.Chapters in books and lectures notes: NA

Conferences:
Poster Presentations

1. 'Mutant p53 affects regulation of survivin by p63', at TMC Platinum Jubilee Conference on New Ideas in Cancer: Challenging Dogmas, Mumbai, India, 2016.
2. ' Role of p63 in regulating p53 repressed proteins survivin and clusterin in human oral cancer' at Gordon Research Conference, June 2014, Vermont, USA.
3. ‘Expression of clusterin and its regulation by p63 in oral cancers’ at the 37th All India Cell Biology Conference, 2013, Bangalore, India.
4. ‘Assessment of p53 family members and survivin isoforms in oral and cervical cancers’ at AACR International Conference, 2011, Delhi, India.

Oral Presentation

- ‘Expression of survivin splice variants and their regulation by p63 in oral cancers’ at 34th Convention of Indian Association for Cancer Research (IACR), 2013, Delhi, India.

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86. Name : **P.V. Srilucksmy**
Enrolment No. : LIFE09200904003
Date of Award of degree : 29.08.16
Constituent Institute : Institute of Mathematical Sciences,
Title : A Study of Spin-Liquids in the Kitaev-Hubbard and Kitaev-Heisenberg Models.

Abstract

The study of spin liquids, an exotic phase of matter, is a rapidly growing field. Spin Liquids are, by definition, pure Mott insulators which, due to quantum fluctuations and frustration, lack magnetic order even at the lowest of temperatures. This exotic behaviour has been observed in a number of materials which include both organic and inorganic salts. It has been possible to classify, using theoretical methods, a total of 180 distinct types of spin liquids. The ground state of one of these, a Z2 type, can be solved exactly. Named the Kitaev spin liquid, this has attracted a lot of attention lately. One of its drawbacks is the sensitivity of the Kitaev model to perturbations that destabilizes the spin liquid phase, letting long-range order set in. This issue, and methods of tackling it, form the backbone of my dissertation.Among the many realisations of the Kitaev spin liquid model, I have chosen to focus on optical lattices and materials. In optical lattice systems, the Kitaev-Hubbard model is defined as a Hubbard model with spin-dependent hopping on a honeycomb lattice. When onsite interactions are large and spin-dependent hopping is strong, The Kitaev-Hubbard model has been shown to host a Kitaev spin liquid model. We have mapped out its phase diagram using numerical techniques such as the Cluster Perturbation Theory (CPT) and the Variational Cluster Approximation (VCA) method. We have detected a new phase where magnetic order is absent but the charge gap is non-zero. We show, using perturbation theory, that spin-spin correlations in this phase decay as a power law. We also show, for the first time ever, that time-reversal symmetry stabilises this new Algebraic Spin Liquid phase.Sodium Iridates Na_2IrO_3 and $Na_4Ir_3O_8$, were proposed to be avenues where Kitaev-like interactions might be realized because of the strong spin-orbit coupling in these 5d-materials. No smoking gun experiment has been found as yet for the detection of spin liquids or of the Kitaev model. Since iridates have recently been shown to possess Kitaev-like correlations, using Raman response as an experimental probe, we analyze Kitaev-Heisenberg model and study Raman responses in depth. Using Majorana mean field decoupling, we show that a broad Raman band at high wavenumbers with weak polarization dependence is a signature for the spin liquid in these compounds.

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1. S. R. Hassan, P.V. Srilucksmy, Sandeep K. Goyal, R. Shankar and David Senechal, ''Stable Algebraic Spin Liquid in a Hubbard model'', PRL, 110, 037201 (2013).
2. P.V. Srilucksmy, Archana Mishra, S.R. Hassan and R. Shankar, "Topological transitions in a model with Particle-Hole symmetry, Pancharatnam-Berry Curvature and Dirac Points", PRB, 89, 045105 (2014).
3. Satyendra Nath Gupta, P.V. Srilucksmy, Kavita Mehlawat, Ashiwini Balodhi, Dileep K. Mishra, D.V.S. Muthu, S.R. Hassan, Yogesh Singh, T.V. Ramakrishnan and A.K. Sood, “Raman

Signatures of strong Kitaev-Exchange correlations in $(Na_{1-x}Li_x)_2 IrO_3$: Experiments and Theory", EPL, 114,47004 (2016).

Sent for Publication

1. Satyendra Nath Gupta, P.V. Sriluckshmy, Ashiwini Balodhi, D.V.S. Muthu, S.R. Hassan, Yogesh Singh, T.V. Ramakrishnan and A.K. Sood, "Spin Liquid like Raman Signatures in hyperkagome iridate $Na_4 Ir_3O_8$ ", Sent for PRB (arxiv:1606.07938.)

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87. Name : **Shiba Prasad Behera**
Enrolment No. : PHYS01201104005
Date of Award of degree : 29.08.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Electromagnetic Simulation of INO-ICAL Magnet and its Sensitivity to Sterile Neutrino Mixing

Abstract

The flagship experiment at the proposed India-based Neutrino Observatory will measure atmospheric neutrinos using the magnetized iron calorimeter (ICAL). The ICAL detector will measure precisely the neutrino oscillation parameters and has the potential of discovering the neutrino mass hierarchy, normal or inverted. The heart of the ICAL detector is ~ 51 kton magnet which will act as a target for the incoming atmospheric neutrinos and identify the neutrino induced charged particles. In this thesis, the design aspects of the ICAL magnet have been investigated by the electromagnetic simulation considering the power efficiency and uniformity of magnetic (B) field within the iron plate. The magnetic field map obtained from the electromagnetic simulation has been used to optimize the B-field strength by studying the muon response. The study of the muon response provides the optimized B-field of about 1.5 T. The muon response has been used to study the active-sterile neutrino mixing sensitivity of ICAL in the '3+1' neutrino mixing frame work. The ICAL detector in the present configuration will be sensitive to the active-sterile neutrino mixing provided the mixing angle $\theta_{24} \geq 10°$ with squared mass difference of $\Delta m^2_{41} \geq 0.1$ eV^2 at 90 % confidence level (C.L.), for the case where neutrinos reach the detector from all directions. By marginalizing over the active-sterile mixing angle and Δm^2_{41}, the upper limit for the mixing angles of θ_{14}, θ_{34} is ~ 20° and for θ_{24} is ~ 12° at 90 % C.L.. Details of the study are presented in thesis.

Publications

Journal

1. Simulation Studies for Electromagnetic Design of INO ICAL Magnet and its Response to Muons, S. P. Behera, M. S. Bhatia, V. M. Datar and A.K. Mohanty, submitted in Trans. Magn., 51, 1 (2015).

Communicated:

1. Physics Potential of the ICAL detector at the India-based Neutrino Observatory (INO), The ICAL Collaboration: Shakeel Ahmed, M. Sajjad Athar, Rashid Hasan, Mohammad Salim, S. K. Singh, S. S. R. Inbanathan, Venktesh Singh, V. S. Subrahmanyam, S. P. Behera et al., arXiv: 1505.07380 (Submitted to PRAMANA).
2. Searching for sterile neutrino mixing with the ICAL detector at INO, S. P.Behera, Anushree Ghosh, Sandhya Choubey, V. M. Datar, D. K. Mishra, and A. K. Mohanty, arXiv: 1605.08607 (Submitted to European Physics Journal C).

Conference Proceedings:

1. Search for sterile neutrino mixing using ICAL detector at INO, S. P. Behera, A. K. Mohanty, Anushre Ghosh, D. K. Mishra, S. Uma Sankar, and V. M. Datar, Proc. of the Symp. on Nucl. Phys., 59, 794 (2014).

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3. Improvements on the Iron Calorimeter Magnet design for INO, S. P. Behera, A. Thirunavukarasu, V. M. Datar, M. S. Bhatia and Y. P. Viyogi; Proc. of the Symp. on Nucl. Phys., 56, 1048 (2011).

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88. Name : **Anil Kumar Soni**
Enrolment No. : ENGG02201104009
Date of Award of degree : 30.08.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Eddy Current Methodologies For Reliable Detection And Rapid Imaging Of Sub-Surface Flaws In Stainless Steel.

Abstract

The conventional eddy current testing is confined to detection of sub-surface flaws within a depth of 5.0 mm in an austenitic stainless steel plate due to the skin-effect phenomenon. Many engineering components are made by austenitic thick stainless steel plates in the range of 8.0 mm to 12.0 mm, such as storage tanks. Due to the presence of hostile corrosive environment, the steel undergoes uniform corrosion, localized pitting and stress corrosion cracking on the inner surface. Inspection of the component surface for corrosion is essential to ensure the structural integrity of the storage tanks. Due to the radiation environment, inspection from inner surface is not possible and detection of inside (deep sub-surface) flaws from outer surface is a challenging application of eddy current testing. Further, rapid automated flaw detection is essential in nuclear industry for ensuring high probability of detection as well as minimal dose of radiation for the inspection personnel. Hence, for reliable detection and rapid imaging of sub-surface flaws in austenitic stainless steel components, development of effective eddy current methodologies is required. This thesis focuses on the design and development of high throughput probes which enable higher strength of the primary magnetic field for deeper penetration of eddy currents into the steel. Finite element modelling based comparative studies have been carried out using COMSOL multi-physics software for selection of optimum coil probe configuration among the send-receive type air core, ferrite core, ferrite core with outer shielding and cup-core probes. This thesis also involves development of a high sensitive eddy current instrument for reliable detection of deep sub-surface flaws. The excitation unit is specially designed to drive a higher excitation current upto 1A into the probe coil and digital lock-in amplifier is designed and implemented using LabVIEW software for precisely measuring the phase lag of the sinusoid from flaws.

To further enhance the detectability of sub-surface flaws with higher signal to noise ratio, this thesis proposes a novel BayWT based image fusion methodology that combines the wavelet transform and Bayesian methodologies. Performance of the proposed fusion methodology is compared with the widely used image fusion methodologies e.g. Laplacian pyramid, wavelet transform, principal component and Bayesian based image fusion. This thesis also proposes a novel scan plan for rapid detection and imaging of flaws which is essential for radioactive environment. For development of the novel scan plan, detailed systematic studies have been carried out for different scan plans viz. raster, diagonal raster, spiral, Lissajous and billiard scan plans. These developed methodologies are applied to 12.0 mm thick AISI type 304L stainless steel plates for detection of flat bottom holes (simulating sub-surface localized corrosion) and EDM notches (simulating sub-surface cracks). The methodologies presented in this thesis demonstrate the synergistic combination of cup-core coil probe and high sensitive instrument for detection of flaws located 8.0 mm below the surface and imaging of flaws using the novel BayWT based image fusion methodology. This study establishes, for the first time, that the billiard scan plan is an attractive scan plan for rapid and reliable eddy current imaging of flaws in large surfaces of electrically conducting materials.

Publications

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1. Anil Kumar Soni, S. Thirunavukkarasu and B. Purna Chandra Rao, ‘Bayes principle based multi-resolution wavelet transform image processing method for enhancement of sub-surface defect images ’, Sensor Review (Under preparation).
2. Anil Kumar. Soni, B. Purna Chandra Rao, S. Mahadevan and S. Thirunavukkarasu, ‘A study on the scan plans for rapid eddy current non-destructive evaluation’, Journal of Nondestructive Evaluation (Under Review).
3. Anil Kumar Soni, B. Sasi, S. Thirunavukkarasu and B. Purna Chandra Rao ‘Development of eddy current probe for detection of deep sub-surface defects’, IETE Technical Review, November 2015, DOI: 10.1080/02564602.2015.1113145.
4. Anil Kumar. Soni, S. Thirunavukkarasu, B. Sasi, B. Purna Chandra Rao, T. Jayakumar, ‘Development of a high sensitive eddy current instrument for detection of sub-surface defects in stainless steel plates’, Insight-Non-Destructive Testing & Condition Monitoring Vol. 57, No. 9, September 2015, pp. 508-512, DOI: 10.1784/insi.2015.57.9.508.
5. S. Thirunavukkarasu, B. Purna Chandra Rao, Anil Kumar Soni, S. Shuaib Ahmed, T. Jayakumar, ‘Comparative performance of image fusion methodologies in eddy current testing’, Research Journal of Applied Sciences, Engineering and Technology, Vol. 4, No. 24, 2012, pp. 5548-5551

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1. Anil Kumar Soni, S Shuaib Ahmed, S. Thirunavukkarasu, B. Purna Chandra Rao and T Jayakumar, ‘Multi-Sensor Image Fusion for Enhanced Detection of Sub-Surface Defects by Eddy Current Testing’, Presented during the 14th Asia Pacific Conference on Non-destructive Testing, Mumbai, 2013.
2. Anil Kumar Soni, B. Purna Chandra Rao, B. Sasi, Saji Jacob George, T Jayakumar, ‘Development of a Low Frequency Eddy Current Instrument for Non-destructive Evaluation’, Presented during the National Symposium on Instrumentation (NSI-38), Hubli, 2013.

Others

1. C.S. Angani, Anil Kumar Soni, K. Sambasiva Rao, Jaskaran Singh Grover, S. Thirunavukkarasu, B. Purna Chandra Rao, T. Jayakumar, 'Development of Pulsed Eddy Current System and Model Based Optimization', Presented during the National Seminar on NDE-2012, New Delhi, 2012.

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89. Name : **Shrichand Jakhar**
Enrolment No. : PHYS06201004001
Date of Award of degree : 31.08.16
Constituent Institute : Institute For Plasma Research
Title : Neutronics Benchmark Studies For The Tritium Breeding Blankets

Abstract

Tritium self-sufficiency is of critical importance to future DT fusion power plants. All DT experimental devices and fusion power plants will have to breed their own tritiumwithlithium containing blankets due to its unavailability in the nature. Nuclear design of the breeding blankets is performed with the neutronics calculations utilizing three dimensional transport codes and cross-section data libraries. The calculated tritium breeding ratio (TBR, ratio of tritium atoms produced in the breeding blankets to that consumed in the plasma) for a given concept of blanket and first wall is uncertain due to uncertainty associated with the system definition and the inaccuracies in predicting the TBR. The latter includes the uncertainty associated with nuclear data, the geometrical modelling, and calculation methods. The calculated achievable TBR in design analyses has to be larger than the required TBR by a margin to safely take into account the uncertainties on the requirements and the uncertainties in design elements, modelling and nuclear data used in the TBR calculations. Therefore, in order to minimize the margins, high accuracy predictions of the TBR and other nuclear responses are needed, which require validated computational tools and qualified nuclear data, including reliable uncertainty estimates. The Fusion Evaluated Nuclear Data Library (FENDL) is widely used worldwide for neutronics calculations in the fusion environment because of the high fidelity of reliability and quality assurance. Despite the high fidelity, the FENDL versions are far from perfect. Integral validation of the data libraries and 3D codes used in the fusion neutronics area is an inevitable step as feedback from integral nuclear testing in a 14 MeV neutron environment leads to significant improvements to cross-section evaluations.The present thesis investigates the nuclear responses of the candidate materials for breeding blankets of a D-T fusion reactor in the form of mock-up assemblies. The measured responses are compared with calculated values obtained from the neutron transport tools used for the nuclear design of the breeding blankets. The main focus of the thesis is to validate the neutron transport physics applied in the calculation tools (code and nuclear data) and to assess the uncertainty in tritium production rate (TPR) due to uncertainty in the relevant nuclear data. The uncertainty in the TPR can eventually be linked to the tritium breeding ratio.India has proposed Lead-Lithium cooled Ceramic Breeder (LLCB) concept of breeding blanket for in-situ tritium breeding in its DEMO reactor. Mock-up of the LLCB breeding blanket will be tested in ITER through Test Blanket Module (TBM) program. A set of four mock-up experiments is evolved during this work to investigate the neutronics performance of materials used in the LLCB TBM. In support of LLCB TBM nuclear design, the first mock-up experimental assembly was designed and fabricated to perform measurements of the nuclear responses. In this thesis, the techniques for the measurement of TPR and neutron flux spectra are developed, characterized and employed in the experimental assemblies containing materials relevant to breeding blankets. Benchmark experiments with three kind of experimentalassemblies are performed and analysed in this thesis. Two experiments are performed with lithium titanate and Lead in the LLCB TBM radial geometry. One experiment was performed with lithium aluminate breeding material. The measured responses are analysed with radiation transport code MCNP using FENDL-2.1 and 3.0 libraries.

The difference between calculated and measured responses with lithium titanate and Lead assemblies is found to be in the range of5-10% due to the nuclear data of the Lead isotopes. Current measurements are also compared with the experiments performed with pure Lead. The impact of the discrepancy in the FENDL nuclear data on the prediction of LLCB TBM breeding performance is discussed.

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Journal

1. “Measurement of tritium production rate distribution in natural $LiAlO_2$/HDPE assembly irradiated by D-T neutrons”,Shrichand Jakhar, M Abhangi, C V S Rao, T K Basu, Sonali P D Bhade, Priyanka J Reddy, *Fusion Eng. Des.,*2012, *87(2)*, 184-187.
2. “Tritium breeding mock-up experiments containing lithium titanate ceramic pebbles and Lead irradiated with DT neutrons”,Shrichand Jakhar, M Abhangi, S Tiwari, R Makwana, V Chaudhari, H L Swami, C Danani, C V S Rao, T K Basu, D Mandal, SonaliBhade, R V Kolekar, P J Reddy, R Bhattacharyay, P Chaudhuri,*Fusion Eng. Des.,*June 2015,*95,*50 - 58.
3. “Neutron flux spectra investigations in breeding blanket assembly containing lithium titanate and Lead irradiated with DT neutrons”,Shrichand Jakhar, S Tiwari, M Abhangi, V Chaudhari, R Makwana, C V S Rao, T K Basu, D Mandal,*Fusion Eng. Des.*, 2015, *100*, 619 - 628.

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90. Name : **Bhanu Prakash Jagilinki**
Enrolment No. : LIFE09200904001
Date of Award of degree : 02.09.16
Constituent Institute : Tata Memorial Centre
Title : Structural and Molecular characterization of an Extracellular signal Regulated Kinase (ERK1/2) in association with Ribosomal S6 Kinases.

Abstract

Cancer is a disease caused by mutations on signaling proteins, thereby deregulating several metabolic pathways. MAPKinase (MAPK) pathway, involving several proteins, is severely deregulated in many known human cancers. The signaling proteins such as Extracellular signal Regulated Kinases and Ribosomal S6 Kinases play major role in cell signaling. Considering the importance of MAPK pathway, structural, biophysical and protein-protein interactions of different domains of kinases proteins have been reported in this thesis. Various techniques such as molecular cloning, protein purification, proteomics, biophysical characterization and bioinformatics have been extensively used to fulfil the objectives set for the Ph.D. thesis.ERK 2 has been purified to study the protein-protein interactions with binding proteins. ITC has been used to quantity the interactions with RSK 3 C terminal synthetic peptide. Further, Protein-protein interactions studiesbetween ERK2 and MEK1, ERK2 and RSK1 have been studied using in-silico molecular docking. Docking studies were performed between ERK2 and C terminal peptides of all RSK 1/2/3/4 isoforms. RSK1 full length protein of 735 amino acids was purified and studied for its biophysical properties. It has been observed that RSK1 is α-helical in nature, however less stable due to its lower T_m. RSK1 CTKD (418-675) was cloned and expressed, and purified from inclusion bodies under denaturing conditions using 8 M urea. Furthermore, RSK3 NTKD and CTKD have been cloned, expressed and purified under the denaturing conditions as they are insoluble. RSK3 CTKD was successfully refolded after screening large number of buffers by trial and error. The refolded RSK3 CTKD was further characterized by various biophysical techniques such as Fluorescence spectroscopy, CD, limited

proteolysis. It was found that the RSK3 CTKD is rich in α-helical content and stable due to high T_m and slow rate of proteolysis. Further DLS studies proved that the RSK3 CTKD exists as trimer in solution. Overall this study further strengthened the understanding of function of MAPK pathways in cell signaling with the emphasis on ERK2 and RSKs, through different biophysical and bioinformatics studies.

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1. Conserved residues at the MAPKs binding interfaces that regulate transcriptional machinery.Bhanu P. Jagilinki,Nikhil Gadewal, Harshal Mehta, HafizaMahadik, Vikrant Pandey, Anamika, UlkaSawant, Prasad A. Wadegaonkar, Peyush Goyal, Satish Kumar & Ashok K.Varma, Journal of biomolecular structure & dynamics,2015,Volume 33, Issue 4, 852–860. doi:10.1080/07391102.2014.915764

2. Functional basis and biophysical approaches to characterize the C-terminal domain of human-Ribosomal s6 Kinase 3. Bhanu P. Jagilinki,Rajan Kumar Choudhary, Pankaj S Thapa, Nikhil Gadewal,M.V.Hosur, Satish Kumar, Ashok K Varma, Cell Biochemistry & Biophysics, June, 2016, pp 1-9, doi:10.1007/s12013-016-0745-6

Under preparation

1. Expression, purification and Biophysical characterization of p90-Ribosomal S6 Kinase- from *Escherichia coli*. Bhanu P. Jagilinki,M.V. Hosur, Ashok K. Varma.

Conferences attended:

1. Indian Association for Cancer Research (IACR), ACTREC, 26-29 January, 2012,.
2. 2nd Global Cancer Genomics Symposium (GCGC), ACTREC, 19-20th November, 2012.
3. International Conference on Structural Genomics 2015 – Deep Sequencing Meets Structural Biology (ICSG2015-DSMSB), Weizmann Institute of Science, Rehovot, Israel,7-11 June, 2015.
4. Indo-French conference on Application of Structural Biology in Translational Research & Structure Guided Drug-Design, ACTREC, 19-20 November, 2015.

91. Name : **Eshita Pal**
Enrolment No. : ENGG01201104016
Date of Award of degree : 08.09.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Simulation And Design Of Passive Moderator Cooling System For Advanced Heavy Water Reactor

Abstract

The Passive Moderator Cooling System (PMCS) of the Advanced Heavy Water Reactor is designed to remove heat from the moderator passively in case of an extended Station BlackOut condition (SBO). The hot heavy-water moderator inside the Calandria rises upward due to buoyancy, cooled in a shell and tube heat exchanger (located within the loop) and returns back to the Calandria, completing a natural circulation loop. The heat exchanger, in turn, is cooled by water from a Gravity Driven Water Pool; forming a second loop. This coupled natural circulation loop system provides sufficient cooling to prevent the moderator temperature inside the Calandria vessel to increase beyond permitted safe limits during SBO.The feasibility of such a system should be assessed before it is implemented in the reactor. Thus, a scaled test facility was designed and built to simulate the thermal hydraulic characteristics of the PMCS. A set of time varying power experiments were performed, which capture the flow initiation from rest phenomena and the multidimensional natural convection flow in a coupled natural circulation system. Next, the experimental geometry was simulated using the three-dimensional computational fluid dynamics code (OpenFoam 2.2.0), which predicted temperature and flow distribution inside the system. The CFD results agree well with the experimental data within ± 6%. To further validate the CFD model, various geometries and flows similar to the PMCS, as available in the published literature were also simulated. Finally, a RELAP5-MOD3.2 simulation of the PMCS for the reactor under prolonged SBO condition was performed. The flow, power and temperature results from this 1D simulation were used as inputs to simulate the 3D CFD model of reactor scale Calandria vessel of the PMCS. The analysis led to the conclusion that the concept of PMCS works, as the system is able to maintain the moderator temperature below boiling conditions for a time period of 7 days without any operator intervention.

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2. “CFD simulations of moderator flow inside Calandria of the Passive Moderator Cooling System of an advanced reactor.”, Pal E., Joshi J. B., Kumar M., Nayak A. K., Vijayan P. K., *Nuclear Engineering and Design*, 2015, *292*, 193-203.
3. “CFD simulations of shell-side flow in a shell-and-tube type heat exchanger with and without baffles.”, Pal E., Kumar I., Joshi J. B., Maheshwari N. K., *Chemical Engineering Science*, 2016, 143, 314-340.
4. “Experimental and CFD Simulations of Fluid Flow and Temperature Distribution in a Natural Circulation Driven Passive Moderator Cooling System of an Advanced Nuclear Reactor.” Pal, E., Kumar, M., Nayak, A.K., Joshi, J.B., *Chemical Engineering Science,* 2016, 155, 45-64.

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2. "CFD Analysis of flow and temperature distribution inside the Calandria of natural circulation, vertical pressure tube type advanced nuclear reactor.", Pal E., Joshi J. B., Nayak A. K., Vijayan P. K., *Fluid Mechanics and Fluid Power-2014.* December'2014. Kanpur, India.
3. "Experimental and Numerical Investigation of Natural Circulation phenomena in a Rectangular Natural Circulation Loop-II.", Pal E., Joshi J. B., Nayak A. K., Vijayan P. K., *Fluid Mechanics and Fluid Power-2014.* December'2014. Kanpur, India.
4. "CFD Analysis of flow and temperature distribution inside the Calandria of Advanced Heavy Water Reactor.", Pal E., Joshi J. B., Nayak A. K., Vijayan P. K., *New Horizons in Nuclear Thermal Hydraulics and Safety.* January'2014. Mumbai, India.
5. "Experimental and Numerical Investigation of Natural Circulation phenomena in a Rectangular Natural Circulation Loop-I.", Pal E., Joshi J. B., Nayak A. K., Vijayan P. K., *New Horizons in Nuclear Thermal Hydraulics and Safety.* January'2014. Mumbai, India.

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92. Name : **Pasula Naresh**
Enrolment No. : ENGG01201104013
Date of Award of degree : 09.09.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Analytical Design And Development Of Resonant Converter Based Fast Capacitor Charging Power Supply (>40 Kj/S).

Abstract

Pulsed power applications usually require short but intense burst of energy that may be delivered by rapidly discharging an energy storage capacitor. To charge this energy storage capacitor a suitable charging source is required. Designing a reliable and efficient charging power supply for pulsed power systems is always a complex job because of associated dynamic load such as electron gun, laser, magnetron etc. During generation and discharge of high intensity pulses the associated charging power supply of pulsed power system undergoes a surge reversal of high amplitude in voltage and high frequency (MHz) noise. To protect the CCPS against this impulse noise, fast protection is needed. Conventionally series resonant converter based CCPS is used for pulsed power applications. But in case of non-linear loading, these CCPS lacks in providing suitable dynamic protection against surge reversal and high frequency noise during discharging period. Other resonant converters such as parallel LC and third order resonant converter have been utilized previously in the development of high voltage CCPS. These power supplies are also suffering with serious issues like lack of DC blocking and poor part load efficiency. An investigation is needed to find out the root cause behind the failure of charging power supply when interfaced with pulsed power system. An attempt has been made to design and develop an efficient and reliable resonant converter based fast (>40kJ/s) CCPS with improved protection for pulsed power applications. A 4th order resonant converter has been proposed and it provides load independent constant current and soft switching when operated at switching frequency equal to resonant frequency. To validate the simulation and mathematical model, a prototype CCPS rated at 200 V, 20 J/s has been developed and load independent constant current is demonstrated with soft switching operation. A high repetition rate CCPS of 4kV, 3.7kJ/s and 9 kHz is designed. High voltage high frequency transformer's leakage inductance is used as one of the resonant inductor. Developed a high charging rate (45 kJ/s) and repetitive (10 Hz) CCPS for 1kJ Marx based system based on 4th order LCLC resonant converter and

successfully interfaced. The failure of controlled switches (IGBTs) in the inverter stage of CCPS due to conducted noise are prevented by effective shielding and proposed LCLC resonant network. With the proposed topology the cost and size of CCPS has reduced due to minimal number of controlled switches, low peak currents and minimum conduction losses in the inverter stage. A photo diode-LED based voltage control circuit has been developed and tested successfully. This control circuit provides more isolation as compared to other electronic components like isolation amplifier and opto-couplers.

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4. Romesh Chandra, A Roy, R Menon, K Senthil, A.S Patel, Igor Ventizenko, A. Mashchennko, Ranjeet Kumar, Tanmay Kolge, Naresh. P, V.K. Sharma, Ritu Agarwal, Archana Sharma and K.C. Mittal "Explosive Emission Properties of Cathode Material in Relativistic Electron Beam Generation" in IEEE Transactions on Plasma Science, Vol. 42, No. 11, November 2014, pp.3491-3497.
5. Naresh P and Archana Sharma, "Analysis and development of 4kV, 9 kHz Repetitive Capacitor Charging Power Supply for Solid State Switch Based Pulsedr Application", in IEEE Transactions on Plasma Science (Major review submitted).

International Conferences papers

1. Naresh. P, Ankur Patel, Tanmay kolge, Ranjeet kumar, Archana Sharma, K.C. Mittal and D.P. Chakravarthy "Voltage Feedback Control for Fast - High Voltage Capacitor Charging Power Supply", Publeshed in 12th International Conference on Electromagnetic Interference and compatibility 2012, INCEMIC – 2012, Bangalore, pp. 64-67.
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4) C S Reddy, Pasula Naresh, Ramanujam Sarathi, Archana Sharma1, Kailash C. Mittal1 “Spark Gap Discharge Properties Measured by Optical Emission Spectroscopy”, 2014 IEEE International power modulator and high voltage conference, 1-5 June,2014, pp. 458-461.
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6) Archana Sharma, Pasula Naresh, Romesh Chandra, K. Senthil, Sabyasachi Mitra, Sandeep Kumar Singh “Characterization of Flash X-Rays Source and Radiography Results of Newly Developed Kali-30GE Relativistic Electron Beam System”, 2014 IEEE International power modulator and high voltage conference, 1-5 June,2014, pp. 370-373.
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National conference

1. Naresh.P, Ankur Patel, Tanmay kolge, Ranjeet kumar, Archana Sharma, K.C. Mittal and D.P. Chakravarthy “Design and Development of Fast - High Voltage Capacitor Charging Power Supply”, Published in VEDA – 2012, Pilani.

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93. Name : **Tanmay Singal**
Enrolment No. : PHYS10200905003
Date of Award of degree : 14.0916
Constituent Institute : Institute of Mathematical Sciences,
Title : Some Problems in Quantum State Discrimination.

Abstract

The problem of Quantum State Discrimination (QSD) is integral to Quantum Information Theory, for e.g. it finds application in many experimental setups which requires one to distinguish among the incoming signal or in the context of communication etc. The basic premise is that one is given an unknown quantum state from a known quantum-state ensemble from which each state can occur with some apriori probability, and one is then tasked with finding which state was given using a quantum measurement. There are many variants of QSD, of which I take up two in this thesis. I consider two problems in each of these variants of QSD, thus four problems totally. The first of these variants is the well known problem of Minimum Error Discrimination (MED) of quantum states. Firstly, I examine the MED problem for ensembles of linearly independent (LI) pure states. While the analytic solution for MED of such ensembles isn't known, the following structure of the problem is known: there exists a bijection from the set of LI pure state ensembles to itself, and this bijection is such that the Pretty Good Measurement (PGM) of the image under this bijection of an ensemble is the optimal POVM for the MED of said ensemble. While the existence of such a bijection is known, its functional form (how it acts on an ensemble of LI pure states) isn't. That said, the action of its inverse is known. I used the implicit function theorem to obtain the solution using the inverse of this bijection. In the second problem I show that this structure (i.e., such a bijection) can be extended to the case of ensembles of LI mixed states, and that this structure can then be subsequently used in the same fashion to compute the optimal POVM for MED of these ensembles. It is seen that this algorithm is as efficient as popular SDP algorithms which are in use to solve this problem. The second variant of QSD concerns the perfect local distinguishability of pairwise orthogonal bipartite quantum states. Firstly, a necessary condition for the local distinguishability of pairwise orthogonal Maximally Entangled States, which goes beyond the known orthogonality preserving condition, is derived. This is done using the Holevo-like upper bound for local distinguishability of ensembles of bipartite states – a result derived by Badziag et al. in Phys. Rev. Lett., vol. 91, p. 117901. It is seen that for sets of *d* MES in *d*x*d* systems, this necessary condition acquires a particularly special form so that it can be checked by solving a set of simultaneous linear equations. This condition is then tested on sets of four MES in 4x4 systems, where these MES are of the form of the Generalized Bell basis states. It is found that for these sets of states this necessary condition is also sufficient to determine the local (in)distinguishability, which shows the strength of this necessary condition. In the next problem I propose a framework for the one-way local distinguishability of sets of pairwise orthogonal states. This is shown through the following sequence of steps: 1.) I borrow a result which states that a set of pairwise orthogonal states is locally distinguishable if and only if the first party can perform an orthogonality preserving rank-one measurement, 2.) I show that the set of orthogonality preserving self-adjoint operators on the first party's side forms a vector space, for which a basis can be constructed, 3.) the existence of an orthogonality preserving rank-one measurement implies and is implied by the existence of a Maximally Abelian Subspace (MAS) in this vector space. Hence I reduce the problem of finding a one-way LOCC protocol to finding a MAS in this vector space. It is shown that the problem of finding such an MAS depends on the dimension of the vector space, for e.g., the result that any two pure states can be perfectly distinguished by one-way LOCC corresponds to the case where the dimension is *d^2-2*. This framework also gives the necessary and sufficient condition for the one-way LOCC distinguishability of almost all sets of *d* orthogonal bipartite pure states. Hence it is argued that a deeper study of this structure is likely to prove rewarding for progress in this topic.

Publications

Journal

1. Minimum error discrimination for an ensemble of linearly independent pure states
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2. Framework for distinguishability of orthogonal bipartite states by one-way local
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94. Name : **Rekha Biswal**
Enrolment No. : MATH10201105001
Date of Award of degree : 14.0916
Constituent Institute : Institute of Mathematical Sciences,
Title : Demazure flags Chebyshev polynomials and mock theta Functions.

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95. Name : **Kamalakshya Mahatab**
Enrolment No. : MATH10201005001
Date of Award of degree : 14.0916
Constituent Institute : Institute of Mathematical Sciences,
Title : Measure Theoretic Aspects Of Error Terms.

Abstract :-

In this thesis, we obtain -bounds for the Lebesgue measure of uctuations of error terms in asymptotic formulas. We also explore the inuence of these bounds on _ estimates of the error terms, which extends Landau's work.The general setup of our methods allow several new applications..

Publications

Journal

1. Kamalakshya Mahatab and Kannappan Sampath, Chinese Remainder The-orem for Cyclotomic Polynomials in Z[X]. Journal of Algebra, 435 (2015), Pages 223-262. doi:10.1016/j.jalgebra.2015.04.006.URL:http://www.sciencedirect.com/science/article/pii/S0021869315001830.
2. Kamalakshya Mahatab, Number of Prime Factors of an Integer. Mathe-matics News Letter, Ramanujan Mathematical Society, volume 24 (2013). URL:https:// mat.iitm.ac.in/home/samy/public_html/MNL-June-13-issue-full 31stJuly13.PDF

Others

1. Kamalakshya Mahatab and Anirban Mukhopadhyay, Measure Theoretic As-pects of Oscillations of Error Terms. arXiv:1512.03144v1 (2015). URL: http://arxiv.org /pdf/1512.03144v1.pdf.

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96. Name : **Anish Mallick**
Enrolment No. : MATH10201104001
Date of Award of degree : 20.09.16
Constituent Institute : Institute of Mathematical Sciences,
Title : Spectral multiplicity for Random Operators with projection valued randomness.

Abstract

The goal of this thesis is to understand the structure of spectrum for certain class of random operators. On

the separable Hilbert space H, the family of operator has the form $A^{\omega}=A+\sum_n \omega_n P_n$, where A is a self-adjoint operator, $\{P_n\}_n$ is a countable collection of rank N projections such that $\sum_n P_n=I$ and $\{\omega_n\}_n$ are real independent random variables with absolutely continuous distribution. One of the important example of these type of random operators is Anderson tight binding model proposed by P. W. Anderson, which is a quantum mechanical model to describe spin wave in doped semiconductor. One of its features is that the singular spectrum is simple. Another operator that is important is random Schrödinger operator, where simplicity of the singular spectrum is still an open problem. This work is an intermediate step in understanding the spectral structure of random Schrödinger operator. Define $\Omega_{n,m}=\{\omega: rank(Q_n^{\omega}P_m)=N\}$, where Q_n^{ω} is the canonical projection onto H_n^{ω}, the closed A^{ω}-invariant subspace containing P_nH. If probability of the events $\Omega_{n,m}$ and $\Omega_{m,n}$ is one, than the absolute continuous part of the positive operator valued measures $P_nE^{\omega}()P_n$ and $P_mE^{\omega}()P_m$ (here $E^{\omega}()$ denotes the spectral measure associated with A^{ω}) are equivalent. Also, the subspaces $E^{\omega}_{sing}H_n^{\omega}$ and $E^{\omega}_{sing}H_m^{\omega}$ are equal, where E^{ω}_{sing} denotes the projection onto the singular subspace of the spectrum for A^{ω}. If probability of the events $\Omega_{n,m}$ and $\Omega_{m,n}$ is one for all n and m, then the singular subspace for A^{ω} is given by $E^{\omega}_{sing}H_n^{\omega}$ for any n

Publications

Journal

1. Mallick, A. (2016), Jakšić–Last theorem for higher rank perturbations. Math. Nachr., 289: 1548–1559. doi:10.1002/mana.201400423.

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97. Name : **Sabeena M.**
Enrolment No. : PHYS02201004004
Date of Award of degree : 26.09.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Phase Transformations in Ti-Mo Alloys.

Abstract

The work presented in the PhD thesis titled "Phase Transformations in Ti-Mo Alloys" submitted by Mrs. Sabeena.M (Enrollment No: PHYS02 2010 04004) for the partial fulfillment of PhD course focuses on the various aspects of diffusional and non diffusional phase transformation in Ti-Mo alloys. A brief discussion about the application of Ti-Mo alloys on various sectors ranging from biomedical to aerospace engineering is described in Chapter 1 in addition to details about alloy classification and the tuning of phase transformation via thermo mechanical treatment and alloying addition. Chapter 2 gives details about the alloy preparations followed by its analysis using experimental and theoretical modeling with a brief overview about the various techniques. Principle, calibration, procedure, source and minimization of errors etc about experimental/computational techniques are discussed. In addition to conventional and Synchrotron XRD, various microscopy techniques like Optical Microscopy (OM), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), and Orientation Imaging Microscopy (OIM) which include Electron Backscatter Diffraction (EBSD) and Precession Electron Diffraction (PED) are discussed. Theoretical method includes DFT, Miedema and JMAT Pro calculations. In Chapter 3, the major part of the study deals with the identification of transformation products with conventional and synchrotron X-ray Diffraction (XRD). In addition to mere identification of crystal structure, detailed Rietveld refinement/DFT calculations has been carried out to retrieve crystal structure details like lattice parameter, atom positions, coordination number, bond length, 3-D strain distribution and the bonding characteristics which are the major theme of Chapter 4. Chapter 5 deals with competing phase transformation mechanisms and products in Ti-1Mo and Ti-7Mo

alloys at various cooling conditions. The thermodynamic basis of the transformation is analysed based on proposed “Free Energy Vs Composition Diagram” and micro structural map. The possibility of variant selection mechanism is analyzed for the same alloys with EBSD/SEM and PED/TEM in the Chapter 6. The signatures of athermal and isothermal ω phase formations, its lattice parameters, the distribution in the β matrix and the lattice collapse mechanism during its formation are discussed in Chapter 7 with an emphasis on the graphite like bonding in the ω phase. Chapter 8 summarizes the findings and novelties of the present study and pointed about the possible scope for further studies.

Publications

Journal

1. “Microstructural characterization of transformation products of bcc b in Ti- 15Mo alloy”,M. Sabeena, Alphy George, S. Murugesan, R. Divakar, E. Mohandas and M.Vijayalakshmi- *Journal of alloys and compounds*, 2016, *658*,301-315.
2. “Thermodynamic basis of non equilibrium phase transformations of bcc- β phase in Ti-Mo system”, M. Sabeena, R. Mythili, Joysurya Basu, and M. Vijayalakshmi,*Transactions of the Indian Institute of Metals,* 2013, 66, 401-407
3. “Studies on ω phase formation in Ti-Mo alloys using Synchrotron XRD”, M. Sabeena, S. Murugesan, R. Mythili, A.K Sinha, M. N Singh, M. Vijayalakshmi, and S. K Deb. *Transactions of the Indian Institute of Metals,* 2015, *68(1)*, 1-6.

Conference presentations

1. “Thermodynamic Basis of Non-equilibrium Phase Transformations of bcc β-phase in Ti-Mo System”, *Presented in ISRS 2012 held at IIT, Madras on Dec 13-15, 2012.*
2. “Influence of Mo in phase stability of Ti-Mo system: Synchrotron based XRD studies”,Presented in *DAE- SSPS* 2013 held at Thapar University, Patiala, Punjab on Dec 17-21,2013.
3. Neutron Activation Analysis of Ti-xMo alloys”, J.S. Brahmaji Rao, M. Sabeena, G. V. S.Ashok Kumar, R. Kumar, M. Vijayalakshmi and C.R. Venkata Subramani, CTAC 2015,May 26-29, at BARC.
4. High Resolution Phase Contrast Microscopy of athermal ω in Ti-15 wt%Mo Alloy”,Alphy George, M. Sabeena, R. Divakar, E. Mohandas and M. Vijayalakshmi, EMSI 2015.

* * *

98. Name : **Ravi Kunjwal**
Enrolment No. : PHYS10201005002
Date of Award of degree : 26.09.16
Constituent Institute : Institute of Mathematical Sciences,
Title : Contextuality beyond the Kochen-Specker theorem

99. Name : **Vikram Singh Dharodi**
Enrolment No. : PHYS06201004004
Date of Award of degree : 26.09.16
Constituent Institute : Institute For Plasma Research,
Title : Collective Phenomena In Strongly Coupled Dusty Plasma Medium.

Abstract

A simplified description of dynamical response of strongly coupled medium is desirable in many contexts of physics. The dusty plasma medium can play an important role in this regard due to its uniqueness, as its dynamical response typically falls within the perceptible grasp of human senses. Furthermore, even at room temperature and normal densities it can be easily prepared to be in a strongly coupled regime. For a strongly coupled medium the slow relaxation effects manifests as visco-elastic behaviour. In the present work the visco-elastic behaviour of the strongly coupled dust fluid has been described by the generalized hydrodynamic (GHD) fluid model. This model introduces strong coupling effects in terms of relaxation parameter τm and the viscosity η. The dynamical response of any medium is best understood in terms of its collective behaviour. We, therefore, focus on the influence of strong coupling on certain collective properties, namely (i) Coherent structures (ii) instabilities and (iii) turbulent transport and mixing within the framework of the GHD model. We have shown numerically, in particular, for the smooth rotating vorticity profile the emission of transverse shear waves traveling with phase velocity as expected analytically from GHD model. It is observed that the existence of transverse shear waves in the GHD fluid significantly modifies the evolution characteristics of coherent structures. Our studies show that due to the existence of such transverse shear waves in the strongly coupled medium, the mixing and transport behaviour in these fluids are much better than in Newtonian hydrodynamic systems. Furthermore, it is demonstrated that the visco-elasticity of the strongly coupled medium leads to a suppression of the Rayleigh-Taylor instability. A conservation theorem has also been constructed, which gives an important tool to have an insight in our system. A detailed numerical simulation studies have been carried out to elucidate this effect.

Publications

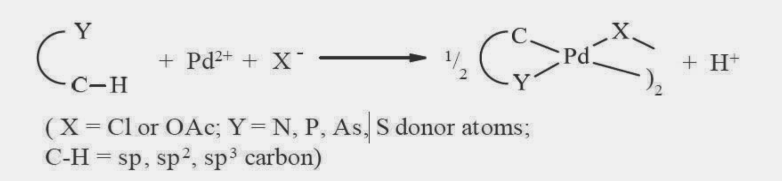
Journal

1. Sub- and super-luminar propagation of structures satisfying Poynting-like theorem for incompressible generalized hydrodynamic fluid model depicting strongly coupled dusty plasma mediumVikram Singh Dharodi, Amita Das, Bhavesh G. Patel and Predhiman Kaw.*Phys. Plasmas 23, 013707 (2016).*
2. Visco-elastic fluid simulations of coherent structures in strongly coupled dusty plasma mediumVikram Singh Dharodi, Sanat Kumar Tiwari and Amita Das.*Phys. Plasmas 21, 073705 (2014).*
3. Collective Dynamics in strongly coupled dusty plasma medium*Amita Das, Vikram Singh Dharodi and Sanat Kumar Tiwari. J. Plasma Physics 80(06), 855- 861(2014).*
4. Kelvin-Helmholtz Instability in dusty plasma medium: Fluid and particle approach*Sanat Kumar Tiwari, Vikram Singh Dharodi, Amita Das, Predhiman Kaw and Abhijit Sen.J. Plasma Physics 80(06), 817- 823(2014).*
5. Effect of strong coupling on the buoyancy-driven instability in strongly coupled dusty plasma mediumVikram Singh Dharodi, Sandeep Kumar and, Amita Das. *To be submitted .*

100. Name **Siddhartha Kolay**
Enrolment No. : CHEM01200904004
Date of Award of degree : 29.09.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Synthesis, characterization and thermal studies of cyclometalated palladium and platinum complexes derived from chalcogen ligands.

Abstract

The chemistry of platinum group metal complexes has witnessed a rapid growth in the last half century owing to the ease of synthesis, rich reaction chemistry and wide applications in diverse areas. Among them cyclometalated compounds represent an interesting family of organometallic compounds [1]. Since the early study of Cope and Siekman in 1965,cyclometalation of organic ligands has emerged as one of the most important reactions in organometallic chemistry and provide a straightforward entry to organometallic compoundsthat feature a metal-carbon σ-bond. The growing interest in these compounds may be attributed to their applications in organic synthesis [2], catalysis (e.g. [Pd2(μ-OAc)2{*o*tol2PC6H4CH2- *o*}2] (*o*-tol = *ortho*-tolyl)) [3], materials science [4] as well as due to their rich reaction chemistry [1]. The cyclometalated complexes are also encountered as reaction intermediates in many organic transformations. Over a period, a myriad of internally functionalized organic compounds containing the neutral donor atom (e.g. N, P, As, O, S) have been utilized for cyclometalation reactions leading to the formation of, in general, a four electron C-anionic donor ligand (C Y). Although several mechanisms have been proposed for the cyclometalation reaction, it is generally believed that initially a ligand is coordinated to the metal centre through a neutral donor atom and in this intermediate species, the C-H bond is activated only when it is within the metal coordination plane (Scheme-1) [5]. Although such intermediates are seldom isolated, their existence can be inferred. X



Scheme 1. Cyclopalladation of organic ligands

The utility of cyclometaladed complexes in materials science, particularly asmesogens,luminescence materials and single source precursors for phase pure inorganic materials, is growing rapidly. The progress for the latter application has however beenhampered due to non-availability of suitable precursors as well as lack of understanding of
thermo-physical properties of such complexes. In view to develop precursors for metachalcogenides, cyclometalation reactions of chalcogen ligands have been investigated and the thermo-physical properties for some representative complexes have been studied during this doctoral program. Among group 16 donors, metalation of oxygen and sulfur compounds are well documented. However, with heavier chalcogen compounds, metalation of only a few organo-selenium ligands (ButSeCH2Ph [6]) has been described recently, whereas there is hardly any report on metalation of tellurium ligands. The thesis is divided into four chapters, *viz.*, introduction, experimental, results and discussion and summary and conclusions, followed by references.

Publications

Journal

1. Binuclear orthometalated N, N-dimethylbenzylamine complexes of palladium(II): Synthesis,structure and thermal behaviorSiddhartha Kolay, N. Ghavale, A. Wadawale, D. Das and V. K. Jain,*Phosphorus, Sulfur, and Silicon and the Related Elements*, 188 (2013) 1449-1461.
2. Cyclopalladation of dimesityl selenide: syntheis, reactivity, structural characterization,isolation of an intermediate complex with C-H…Pd intra-molecular interaction andcomputational studiesSiddhartha Kolay, A. Wadawale, D. Das, H. K. Kisan, R. B. Sunoj and V. K. Jain, *DaltonTrans.*, 42 (2013) 10828-10837.
3. Cyclopalladation of telluro ether ligands: Synthesis, reactivity and structural characterizationSiddhartha Kolay, M. Kumar, A. Wadawale, D. Das and V. K. Jain,*Dalton Trans.,* 43 (2014) 16056-16065.
4. Role of anagostic interactions in cycloplatination of telluro ethers: Synthesis and structuralcharacterizationSiddhartha Kolay, M. Kumar, A. Wadawale, D. Das and V. K. Jain,*J. Organometal. Chem.*, 794 (2015) 40-47.
5. Platinum mediated activation of coordinated organonitriles by telluroethers in THF: Isolation,structural characterization and DFT analysis of intermediate complexes Siddhartha Kolay, A. Wadawale, S. Nigam, M. Kumar, C. Majumder, D. Das and V. K. Jain,*Inorg. Chem.* 54 (2015) 11741–11750.
6. Synthesis, structures and thermal behaviour of cyclopalladated 1,1-dithiolatecomplexesSiddhartha Kolay, A. Wadawale, D. Das and V. K. Jain,Manuscript under preparation.

Conferences

1. Cyclopalladation of telluro ether: Synthesis and structural investigation\Siddhartha Kolay, M. Kumar, A. Wadawale, D. Das and V. K. Jain5th Interdisciplinary Symposium on Materials Chemistry, December 9-13, 2014, BhabhaAtomic Research Centre, Mumbai, Page: 460.
2. Cyclometalation of seleno and telluro ether ligandsSiddhartha Kolay, A. Wadawale, D. Das and V. K. JainNational Conference on Chemistry of Chalcogens and Related Type equation here.Topics (NC3-2015), DefenceInstitute of Advanced Technology (DIAT), Pune; 12-13 January, 2015.
3. Synthesis and thermochemical studies of platinum group metal complexes derived fromorganochalcogen ligandsSiddhartha Kolay and D. Das27th Research Scholars Meet-2015; Indian Chemical Society (Mumbai Branch) and SathayaCollege, Mumbai, 20-21 February, 2015.

101. Name : **Aravapalli Shriniwas Rao**
Enrolment No. : ENGG01200904025
Date of Award of degree : 29.09.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Modeling Of Agitated Bunsen Reactor For Iodine Sulfur Thermochemical Process For Production Of Hydrogen With Experimental Validation

Abstract

The problem definition, pointing out the research gap on information on Bunsen reaction and simultaneous phase separation in single equipment by citing appropriate references has been presented and a new counter-current reactor concept has been proposed to implement the Bunsen reaction and phase separation.Experimental techniques and methods used in the research work have been described. Analytical methods for analysis of H^+, $HI(I^-)$, I_2, KOH and NaCl in sample has been described along with the static mixer reactor and agitated Bunsen reactor used in the study. Reaction studies in static mixer reactor and modeling has been detailed. Experiments with pure SO_2 & N_2 were carried out to study the effect of temperature and pressure on reaction length. Also, experiments were carried out with SO_2 and N_2 mixture to analyze the effect of gas film resistance. It was concluded that for Iodine-Sulfur thermo-chemical cycle, the effect of temperature is predominant on reaction length or reaction rate when compared with that of effect of pressure.Results of Residence Time Distribution (RTD) studies for Agitated Bunsen Reactor (ABR) have been discussed. Dispersion model for small and large extents of dispersion was used for calculating dispersion coefficient. RTD studies in ABR was identified, to have importance in identifying the agitation speed for plug flow regime in tubular reactor with an agitator inside. Effect of variation of agitation speed and water flow rate in ABR, with water as reactor fluid and NaCl as tracer was studied experimentally.For heat transfer based preliminary design of ABR, the analysis of operating parameters on heat transfer and correlations were developed. In ABR heat removal can be more efficient by increasing the agitation speed and cooling water flow rate through the coil. Modified heat transfer correlations proposed was found reasonably accurate in the flow Reynold's number range of 50 to 500 and impeller Reynold's number of 1,500 to 15,000.The phase separation studies in ABR have been carried out. Two different pairs of chemicals "water and kerosene" and "Hydriodic acid and sulphuric acid" were used. Separation behaviour of counter current flow reactor at different flow rates and different agitation speeds were studied. It was concluded that process integration, Bunsen reaction and separation of phases in single equipment is feasible.The Bunsen reaction and layer separation of product acids viz. sulfuric acid and hydriodic acid have been studied in ABR. Experiments with pure and dilute SO_2 were conducted to study the effect of flow rate, reactor temperature and partial pressure. It was observed that density of layer separated bottom heavy phase was less affected by different experimental condition and top light phase have significant change with experimental condition.The mathematical model has been proposed for ABR to predict reaction rate and conversion for the experiments, performed at different temperature by varying SO_2 partial pressure with different combinations of N_2. Results obtained from experiments were compared with theoretical predictions and are found to be in agreement thus validating the proposed model for agitated Bunsen reactor system.

Publications

Journal

1. "Study of effect of high Pressures and elevated Temperatures on Bunsen reaction of Iodine-Sulfur thermo-chemical proce ss" A Shriniwas Rao, S. Sujeesh, V. Nafees Ahmed, H Z Fani, P K Tewari, L M Gantayet, International Journal of Hydrogen Energy, 2015, 40 pp 5025-5033.
2. "Study of Bunsen reaction in Agitated reactor operating in counter current mode for Iodine-Sulfur thermo-chemical process" A Shriniwas Rao, S Sujeesh, V Nafees Ahmed, H Z Fani, A

Sanyal, P K Tewari, L M Gantayet, International Journal of Nuclear Hydrogen Production and Applications, Vol. 3, No. 1, 2016, pp 12-31.

3. “Effect of agitation speed and fluid velocity on heat transfer performance in agitated Bunsen Reactor of Iodine-Sulfur thermo chemical cycle” A Shriniwas Rao, S Sujeesh, A Sanyal, P K Tewari, L M Gantayet, International Journal of Nuclear Hydrogen Production and Applications, Vol. 3, No. 1, 2016, pp 65-79.

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102. Name : **Soumitra Kar**
Enrolment No. : ENGG01201204011
Date of Award of degree : 07.10.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Development Of Nanocomposite Membranes For Enhanced Performances

Abstract

The thesis entitled “Development of Nanocomposite Membranes for Enhanced Performances” deals with facile development, in-depth studies and extensive investigation as well as performance evaluation of a series of polymer–inorganic nanocomposite membranes, all of them being of mixed-matrix ultrafiltration (UF) type. The work was undertaken keeping in to context the necessity of development of enhanced-performance, novel membrane materials as a crucial step towards a sustainable societal and industrial growth. To appreciate the effect of different nanomaterials, the polymer through-out the research work has been kept the same, that is Polysulfone (Psf) and the membranes were prepared by phase inversion technique. There are four different objectives with which the experimental investigations were carried out based upon the functional advantages offered by the nanomaterials. The first study was aimed at development of a membrane to result in minimization of trade-off between flux and selectivity upon impregnation of reduced graphene oxide (RGO) onto Psf host matrix. Studies revealed that an optimum loading of RGO (2 % of polymer weight) in the Psf matrix resulted in membranes with enhanced permeability (4200 LMD and improved rejection attributes (92 % against polyethylene glycol of 35 kDa) compared to pure Psf membrane (Flux: 3700 LMD; Rejection: 65 %). The second study was aimed at development of membranes with improved biofouling resistance properties. Silver nanoparticles and carbon nanotubes (CNTs) were taken up for composite fabrication in this case. It is confirmed that incorporation of silver (1 % of polymer weight) not only results in a bio-fouling resistant membrane, but also silver has got a pronounced role to play in bacterial rejection only when the membrane matrix is sufficiently porous (~80 %). The experimental output and the idea was utilized to develop a process know-how for a domestic water purification device with about 6 times enhanced flux (compared to conventional UF based domestic water purifier) and 99.99 % bacterial decontamination. On the other hand, it was observed that impregnation of CNTs (single/multi walled) does not help reasonably in making the membrane biofouling resistant, which could be because of misalignment of CNTs during the membrane preparation. The third study was aimed at development of membranes with improved radiation resistance properties. Pyrochlore ($Gd_2Zr_2O_7$) was chosen for composite membrane making along with Psf. The extent of damage caused due to 1000 kGy gamma irradiation (correlated with the extent of reduction in elongation at break values) is about 90 % for pure Psf whereas the membranes with 2 % nanoparticle loading showed only about 57 % reduction in elongation at break, which resulted in a membrane with improved radiation resistance behaviour of all the membrane samples prepared. However, from membrane performance perspective, 1 % pyrochlore loaded mixed matrix membrane showed the optimum flux behaviour without compromise in selectivity and tensile strength. Lastly, attempts were made to develop mixed-matrix UF membranes with superior transport characteristics and stimulating antifouling activity by impregnating organofunctionalized (sulfonated) TiO_2 and carboxylated CNTs. The sulfonated TiO_2 embedded membranes exhibited high solvent throughputs (2 times that of control Psf membranes) without notable reduction in their solute rejection capabilities. The flux recovery ratios and fouling resistive behaviors of the membranes towards bovine serum albumin (BSA) solution confirmed that the enhanced hydrophilicity and strong long-range repulsive forces (induced by sulfonated TiO_2) impart stable and extensive antifouling activity onto the membrane surface. It is observed that though the incorporation of CNTs onto Psf hardly leads to any improvement in flux and rejection behaviour, the incorporation of charged (carboxyl acid group) CNTs leads to a 1.5 to 2 times flux enhancement (Psf membrane: 2880 LMD; Nanocomposite Psf: 4320 to 5760 LMD) without compromise in the solute rejection abilities (about 90 % solute rejection against polyethylene oxide of 100 kDa) of the membranes. The thesis at the end recommends for fabrication and usage of surface located nanocomposites for better exploitation of nanostructured materials.

Publications

Journal

1. Charged thin film composite nanofiltration membrane and process of its production; Patent Inventors: T. K. Dey, Avishek Pal, R. C. Bindal and P. K. Tewari Indian Patent Application No.: 1902 / MUM / 2014, filed on June 10, 2014.
2. Nanofiltration membranes with surface negative charge for fractional separation of mono and multivalent ionic species; Patent Inventors: T. K. Dey, Avishek Pal, R. C. Bindal and P. K. TewariIndian Patent Application No.: 2095 / MUM / 2015, filed on May 29, 2015.

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103. Name : **Rishi Pamnani**
Enrolment No. : ENGG02201204013
Date of Award of degree : 07.10.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Effect of Arc Welding Processes on the Weld Attributes of Micro Alloyed HSLA Steel

Abstract

The primary aim of the investigations carried out in the PhD was to study feasibility of activated flux gas tungsten arc welding (A-GTAW) process as alternate welding technique for naval structural steel (DMR-249A) and compare the effect of different arc welding processes on weld attributes of DMR-249A steel weld joints. The experiments were carried out with combinations of oxide fluxes to develop suitable activated flux for GTAW of DMR-249A steel. The bead width and depth of penetration obtained in the bead on plate experiments using various combinations of fluxes were measured. Mixture 1, with maximum depth to width ratio about 0.86, was used as optimum flux combination to carry out experiments for optimising welding parameters.Design of Experiments (DOE) approach was employed using Response Surface Methodology (RSM) and Taguchi technique to optimize the welding parameters for achieving maximum Depth of Penetration (DOP) in a single pass. Design matrix was generated using DOE techniques and bead on plate experiments were carried out to generate data regarding influence of welding process variables on DOP. The input variables considered were current, torch speed and arc gap and the DOP was considered as the response variable. The equations correlating depth of penetration with the process parameters were developed for both the optimization techniques. The identified optimum process parameters were validated by carrying out bead on plate experiments. The root mean square (RMS) error between the predicted and measured DOP values for the validation experiments of the RSM (D-Optimal) and Taguchi optimization technique was found to be 0.57 and 0.86 respectively. Thus, RSM (D-Optimal) was observed to predict optimized welding process parameters for achieving maximum DOP with better accuracy during A-GTAW process. The welding parameters of 270 A current, 60 mm/min speed and 3 mm arc gap were finalised to

carry out double sided A-GTAW weld joint.Four weld joints were fabricated using shielded metal arc welding (SMAW),submerged arc welding (SAW), flux cored arc welding (FCAW) and activated flux gas tungsten arc welding (A-GTAW) processes.All the four weld joints passed radiographic examination. The Finite Element Model (FEM) simulation of thermo-mechanical behavior of SMAW (the most common welding technique used for welding of microalloyed steels and construction of ships) and A-GTAW (welding technique being studied and developed as alternative welding technique for DMR-249A steel) joints was studied using SYSWELD software. The double ellipsoidal heat source distribution model was employed for the thermal and residual stress analysis. The numerically estimated temperature distribution was validated with online temperature measurements using K-type thermocouples. The predicted residual stress profiles across the weld joints were compared with the values experimentally measured using non-destructive techniques. X-Ray Diffraction (XRD) and ultrasonic technique (UT) were used to experimentally estimate the residual stresses across the weld joints. The residual stresses profile of higher heat input A-GTAW process was observed to be comparable with SMAW process. A good agreement between measured and predicted thermal cycles and residual stress profile established FEM as a dependable technique to estimate residual stresses in arc welded joints of DMR-249A steel.The microstructure study of the base metal DMR 249A and the four weld joints were undertaken using optical microscope, SEM and EBSD. The microstructure of DMR-249A steel exhibited predominantly fine grained equiaxed ferrite and some percentage of pearlite of banded type structure. For weld metals, the optical micrographs showed grain boundary ferrite, Widmanstatten ferrite with aligned second phase along with veins of ferrite, acicular ferrite, polygonal ferrite and microphases. The minor changes in percentage of volume fraction of the different ferrites (grain boundary, Widmanstatten, acicular and polygonal) were observed in the samples characteristic to the difference in heat input of the various arc welding processes. The inclusion rating and estimation of volume fraction of various ferritic morphologies was undertaken to correlate microstructural transformation during welding with mechanical properties of various arc welded joints. The hardness values measured across the weld joints were found within the scatter band of 200 -290 $HV_{0.2}$ as compared to values of 196-210 $HV_{0.2}$ for base metal. The hardness of weld metal was observed to be higher than the base metal. The micro-hardness values gradually increases from base metal to HAZ and a minor decrease in the hardness value was observed near the fusion zone followed by higher hardness values in weld metal. Similar trends of hardness values have been reported in weld joint of HSLA steels.The investigations were carried out to ascertain the mechanical properties of the weld joints. The tensile test performed on base metal and cross weld joint specimen showed higher yield strength about 460 - 480 MPa in the cross weld joints as compared to about 427 MPa of base metal. The percentage elongation of cross weld joint (19-20%) was lower than the base metal (30%). The UTSof both the base metal and weld joints were comparable (about 600 MPa). The tensile fracture of the cross weld joint occurred in the base metal region away from weld metal which confirmed the existence of adequate strength in weld metal. The A-GTAW process being the newly developed welding process for DMR-249A steel, 180° bend test was carried out only for A-GTAW joint. No cracks observed on application of dye penetration testing confirmed the integrity and adequate ductility of A-GTAW weld joint.The impact toughness values of base metal (>350 J and 160 J respectively at room temperature and -60°C) was observed to be superior than the weld joints (160-200 J and 10-70 J respectively at room temperature and -60°C). The difference in impact toughness values is attributed to presence of impurities/inclusions in weld metal, coarse grain size due to welding heat input and traces of grain boundary and Widmanstatten ferrites in weld metal as compared to smaller equiaxed grains of base metal.The mechanical properties across the SMAW, SAW, FCAW and A-GTAW weld joints in DMR-249A steel were evaluated using automatic ball indentation (ABI) technique. The tensile strength was observed to vary significantly across the weld joints. The strength values (YS and UTS) decreased systematically across the weld joint from weld metal to base metal. The strain hardening exponent was found to be comparable across the weld joints with marginal higher values for HAZ. The comparable values of strain hardening exponent for weld metal and base metal showed the balanced strength and ductility of the welds. The ABI was found to be a dependable technique for analysis and characterization of mechanical properties across weld joint by using a small amount of test materials.The electrochemical properties of base metal (DMR-249A HSLA steel) and welded butt joints were compared by conducting potentiodynamic anodic polarization studies. Experiments were also carried out with base material samples of ABA and D40S steels for comparing and understanding corrosion behaviour of DMR-249A steel. The base metal and weld metals of arc welded joints displayed similar corrosion characteristics for general and pitting corrosion in sea water and fresh water. It was concluded that the qualified arc welding processes did not deteriorate the corrosion characteristics of the base metal, DMR-249A steel.The values of hardness and strength exhibited by A-GTAW weld metal were comparable with weld metals of other arc welded joints. The A-GTAW weld joint indicated good impact toughness value of 200 J at room temperature. The sub zero (-60°C) impact toughness was found to be 10 J. The significant reduction in toughness of A-GTAW joint at sub-zero temperatures is attributable to more percentage of grain boundary ferrite and Widmanstatten ferrite in high heat input double pass A-GTAW welding process. The coarse grains of A-GTAW weld metal is also a significant factor leading to decrease in sub-zero impact toughness.The weld attributes of phase transformation, microstructure, inclusions and mechanical properties were found to be distinctive characteristic of the different arc welding processes studied. The hardness, tensile properties and corrosion properties were found to be comparable for all the weld joints. The FCAW and SMAW joints exhibited better sub-zero impact toughness followed by SAW and A-GTAW.The significant variation observed in sub-zero impact toughness was attributed to the microstructral transformation of equiaxed base metal to various ferrite morphologies, grain size, inclusions and variation in chemical composition of weld metals of different joints.

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Journal

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2. Rishi Pamnani, R.P. George, B. Anandkumar, T. Jayakumar, M. Vasudevan, U. Kamachi Mudali. Electrochemical Corrosion Studies Of Base Metals And Welds Of Low Carbon Steels Used In Ship Building Industry: Innovations In Corrosion And Mat. Sc, Bentham Publication, Vol 6, DOI: 10.2174/2352094906666151207195150
3. Rishi Pamnani, Govind K. Sharma, S. Mahadevan, T. Jayakumar, M. Vasudevan, B.P.C. Rao. Residual Stress Studies On Arc Welding Joints Of Naval Steel (DMR-249A): Journal Of Manufacturing Processes, 20 (2015), 104-111.
4. Rishi Pamnani, M Vasudevan, T Jayakumarand P Vasantharaja. Development Of Activated Flux, Optimization Of Welding Parameters And Characterization Of Weld Joint For DMR-249A Shipbuilding Steel: Trans IIM, 2016, DOI: 10.1007/S12666-016-0857-0
5. Rishi Pamnani, M Vasudevan, T Jayakumar, K C Ganesh, P Vasantharaja. Numerical Simulation And Experimental Validation Of Arc Welding Of DMR-249A Steel: Defence Technology, 12 (2016), 305–315
6. Rishi Pamnani, T Jayakumar, M Vasudevan, T Sakthivel. Investigations On The Impact Toughness Of HSLA Steel Arc Welded Joints. Journal Of Manufacturing Processes, 21 (2016), 75–86
7. Rishi Pamnani, V Karthik, T Jayakumar, M Vasudevan And T Sakthivel. Evaluation Of Mechanical Properties Across DMR-249A Steel Weld Joints Using Automated Ball Indentation.Materials Science&Engineeringa, 651(2016), 214–22.
8. Rishi Pamnani, T Jayakumar, M Vasudevan, V Shankar, P Vasantharaja. Effect Of Arc Welding Processes On The Microstructure And Mechanical Properties Of Naval Steel (DMR-249A) Weld Joints: Defence Technology- DT-D-16-00017

Conferences Attended

1. Development Of Improved Welding Technique For Naval Structural Material (DMR-249A). Rishi Pamnani, T Jayakumar, M Vasudevan, P Vasantharaja, IWCEM-2014, Pune, 24-26 May 2014.

2. Optimising Welding Of Naval Construction Steel By Design Of Experiments. Rishi Pamnani, T Jayakumar, M Vasudevan, P Vasantharaja, IWCEM-2015, Pune, 23-25 May 2015.
3. Studies On Corrosion Characteristics Of High Strength Low Alloy Steels Used In Ship Building Industry. Rishi Pamnani, B Anandkumar, RP George, T Jayakumar,M Vasudevan,U Kamachi Mudali,IWCEM-2015, Pune, 23-25 May 2015.
4. Electrochemical Potentiodynamic Studies Of High Strength Low Alloy (HSLA) Marine Steels. Rishi Pamnani, B Anandkumar, RP George, T Jayakumar,M Vasudevan,U Kamachi Mudali,CORSYM-2015, Chennai, 31 Jul-01 Aug 2015

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104. Name : **T.R. Devidas**
Enrolment No. : PHYS02201004006
Date of Award of degree : 07.10.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Magneto-transport and High Pressure transport studies on the Topological Insulator system Bi2Se3.

Abstract

The work presented in the PhD thesis titled “Magneto-transport and High Pressure transport studies on the Topological Insulator system Bi_2Se_3” focuses on the low temperature transport properties of single crystals of the Topological Insulator (TI) system Bi_2Se_3 under magnetic fields in the range of 0 – 15 T and under high pressure in pressure range of 0 – 8 GPa. Chapter 1 gives a brief introduction to the field of TI and the challenges present in measuring transport from the Topological Surface States (TSS) such as Shubnikov de Haas oscillations (SdH) in them, in particular the Bi_2Se_3 system. The thesis aims at understanding the role of defects and disorder on the transport properties of topological insulator (TI) system Bi_2Se_3. Chapter 2 deals with the various experimental techniques used in the current thesis viz., Powder XRD, Laue diffraction, High Pressure resistivity, Magneto-transport measurements and Positron Lifetime spectroscopy technique. Chapter 3 focuses on studying the role of defects in achieving Quantum oscillations in magneto-transport from surface states by introducing weak and strong disorder by varying the growth conditions of Bi_2Se_3 single crystals. It is observed that Se vacancies play the prominent role in n-type doping of the bulk and the appearance of Shubnikov-de Haas (SdH) oscillations in Bi_2Se_3 is directly correlated to the presence of low-angle grain boundaries and extended defects such as stacking faults in Bi_2Se_3, that shift the Dirac point to lower energies leading to upward band-bending behaviour, which in turn favour the transport being dominated by the TSS [*EPL* 108 (2014) 67008]. Chapter 4 deals with the effect of Sb substitution at Bi site in Bi_2Se_3 [$Bi_{2-x}Sb_xSe_3$ (x = 0, 0.05, 0.1, 0.3, 0.5)], on the transport from TSS. Sb substitution at Bi site is predicted to reduce the bulk band gap in the system. With increase in Sb substitution, it is observed that the origin of the SdH oscillations changed from the TSS to a conventional 2DEG that arises because of downward band-bending occurring in the system [unpublished]. Chapter 5 deals with the effect of Te substitution at Bi site in Bi_2Se_3 [$Bi_2Se_{3-x}Te_x$ (x = 0, 1, 1.8, 2)], on the transport from TSS. Te substitution at Se site in samples introduces very strong electronic disorder driving the bulk into highly localised state, hence leading to observation of Weak Anti-Localization [WAL] phenomena, a signature of TSS in magneto-resistance measurement. The Hall slope too exhibits non-linear behaviour indicative of TSS contribution in transport [*J. Phys.: Condens. Matter* 28 (2016) 075003]. In Chapter 6, high pressure resistivity measurements are carried out on Te substituted Bi_2Se_3 [$Bi_2Se_{3-x}Te_x$ (x = 0, 1, 2, 3)] system. It is observed that while Bi_2Se_3 shows increasingly non-metallic behaviour [*AIP Conf. Proc.* 1512 (2013) 964], the Te substituted samples are driven into a superconducting phase with pressure with transition temperature in the range of 6±2 K. The nature of the pressure induced superconducting phase was found to be of conventional BCS type and the analysis of the normal state resistivity at critical pressure suggests that the pressure induced superconductivity in this system may lie in the regime of weakly coupled superconductors [unpublished]. Chapter 7 summarizes the results from the previous chapters and also gives an outlook towards the future work that can be carried out in the system.

Publications

Journal

1. Role of Se vacancies on Shubnikov-de Haas oscillations in Bi2Se3: A combined magneto-resistance and positron annihilation study T. R. Devidas, E. P. Amaladass, Shilpam Sharma, R. Rajaraman, D. Sornadurai, N. Subramanian, Awadhesh Mani, C. S. Sundar and A. Bharathi, *EPL* 108 (2014) 67008
2. Magneto-transport behaviour of Bi2Se3-xTex: Role of disorder E. P. Amaladass, T. R. Devidas, Shilpam Sharma, C. S. Sundar, Awadhesh Mani and A. Bharathi, *J. of Phys.: Condens. Matter* 28 (2016) 075003.

Manuscript under revision:

1. Magneto-transport in the Topological Insulator system Bi2-xSbxSe3T. R. Devidas, E. P. Amaladass, Shilpam Sharma, Awadhesh Mani, R. Rajaraman, C.S. Sundar and A. Bharathi.

Other Publications

1. Pressure-induced structural changes and insulator-metal transition in layered bismuthtriiodide, BiI3: a combined experimental and theoretical studyT. R. Devidas, N. V. C. Shekar, C. S. Sundar, P. Chithaiah, Y. A. Sorb, V. S.Bhadram, *Journal of Physics: Condensed Matter* 26 (2014) 275502
2. Observation of superconductivity in SrMnBi2 and Bi interfaceK. Vinod, A. Bharathi, A. T. Satya, Shilpam Sharma, T. R. Devidas, AwadheshMani, A. K. Sinha, S. K. Deb, V. Sridharan, C. S. Sundar, *Solid State Commun.* 192(2014) 60
2. Unification of the pressure and composition dependence of superconductivity in Rusubstituted BaFe2As2 T. R. Devidas, Awadhesh Mani, Shilpam Sharma, K. Vinod, A. Bharathi, C. S. Sundar, *Solid State Commun.* 185 (2014) 62.

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1. High pressure studies on topological insulator Bi2Se3T. R. Devidas, Awadhesh Mani, and A. Bharathi, *DAE-Solid State PhysicsSymposium (DAE-SSPS, December 3-7, 2012)* Mumbai, India Published in *AIP Conf. Proc.* 1512 (2013) 964.
2. Polarized Micro-Raman spectra of Sb2Te3: A Topological Insulator T. R. Devidas, S. Dhara, Awadhesh Mani, A. Bharathi, *International Conference OnRaman Spectroscopy (ICORS, August 12-17, 2012)* Bangalore, India.

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105. Name : **Amit Dutta Banik**
Enrolment No. : PHYS05201004004
Date of Award of degree : 07.10.16
Constituent Institute : Saha Institute of Nuclear Physics,
Title : Study of different Dark Matter models with extended Higgs Sector.

Abstract

Existence of dark matter have already been established by different astrophysical evidences such as rotation curve of spiral galaxies, study of cosmic microwave back-ground radiation etc. However, particle nature of dark matter still remains unknown .Till date ongoing direct detection experiments have not detected any signal of dark matter-nucleon scattering from their direct search experiments. Indirect

searches for dark matter are also performed searching for excess in gamma-ray, neutrino flux etc.by different earth based and satellite borne experiments. In this work, different mod- els for particle dark matter candidate are proposed. These proposed dark matter models are then constrained by different theoretical and experimental bounds to find out the available model parameter space. First, we briefly discuss the physics of darkmatter and Standard Model (SM) of particle physics. A model for fermionic darkmatter in two Higgs doublet model is then worked out. The fermionic dark matter candidate is stabilised by a discrete Z'_2 symmetry. The viable model parameter space consistent with Planck dark matter relic density, direct detection experiments etc. is obtained. In the next work, an extension of inert doublet model (IDM) with ad-ditional singlet scalar is performed. Phenomenology of the model is presented and also study of Higgs to diphoton channel in the present model has been pursued. Werestrict the usual dark matter model parameter space with the signal strength of Higgs to diphoton channel and a region of allowed low mass dark matter of mass $m \leq 80$ GeV have been found. In an another work, the same model is used to carry out indirect detection studies to find out whether the existing model is good enough to fit with 1-3 GeV gamma-ray excess at galactic centre observed by Fermi-LAT. We found that a 31- 40 GeV dark matter can fit the experimental observations withsinglet scalar having mass $\sim$ 70 GeV. In the final work a hidden sector dark mattermodel is proposed where the lightest fermion in the hidden sector is a viable can-didate for dark matter. The parameter space of the hidden dark matter scenario iscon strained by several theoretical and experimental bounds and valid model parame-ter space is obtained. Viability of the model is further tested by the study of galacticcenter (GC) gamma ray flux obtained from updated analysis of Fermi-LAT data ofGC gamma ray. We show that the available model parameter space of hidden sector fermionic dark matter can indeed explain the updated gamma-ray results from GC, dwarf galaxy gamma ray flux results. Finally, a direction of future work have been discussed briefly to conclude the dissertation.

Publications

Journal

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3. Low Energy Gamma Ray Excess Confronting a Singlet Scalar Extended InertDoublet Dark Matter Model A. D. Banik and D. Majumdar Phys. Lett. B 743 (2015) 420, [arXiv:1408.5795 [hep-ph]].
4. Possible Explanation of Indirect Gamma Ray Signatures from Hidden Sector Fermionic Dark Matter A. D. Banik, D. Majumdar and A. Biswas Eur. Phys. J. C76 (2016) 346, [arXiv:1506.05665 [hep-ph]].

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106. Name : **Sadu Venkatesu**
Enrolment No. : ENGG02201004006
Date of Award of degree : 07.10.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Design And Development Of Out-Of-Pile Version Of Instrumented Capsule For Online Determination Of Uniaxial Creep Behavior In Structural Specimen.

Abstract

The experiments had been carried out with focus towards design and development of instrumented capsule for determination of uniaxial creep behavior in structural specimen. Analytical calculations and design have been carried out, the bellows setup has been fabricated through the industry. These bellows have been tested under cyclic load and found to be performing satisfactorily then fabricated an out-of-pile version of instrumented capsule. Argon at a pressure of 6.0 MPa has been filled in the capsule and sealed to apply a nominal load on the tensile specimen at room temperature. The instrumented capsule has been kept in the electric furnace and the temperature of furnace is raised. As the temperature of the furnace rises, the pressure of gas increases leading to increased load on the specimen. For validating the design concepts, these experimental results have been compared with obtained literature results. Force/ load due to argon gas pressure is the major component for the tensile loading of the specimen. The 95% of the total load is acting on the specimen and remaining 5% load only is acting on the bellow. Experimental results (steady state creep values) have been compared with the literature results, and found to be closely matching. Design concept of instrumented capsule for uniaxial creep measurement has been validated. The design of instrumented capsule is directly applicable for in-reactor experiments of a fast reactorHeat transfer analysis of irradiation capsule by an analytical and simulation techniques has been carried out. In a nuclear reactor, structural material specimens are subjected to irradiation to determine the changes in their mechanical properties due to exposure to radiation. In one of the types of irradiation capsules, the specimens are kept in four to five separate sealed compartments of the capsule located one over the other. Helium/ Argon gas or mixture of these gases will be filled around the specimens in these compartments. Liquid sodium, which is the coolant in the reactor, will be flowing around the irradiation capsule. During irradiation, due to attenuation of gamma rays and neutrons on the specimens, heat will be generated in the specimens. Due to this, the temperature of the specimens will be more than the temperature of the sodium flowing over the capsule and we can obtain an irradiation temperature in the specimens which is higher than the sodium temperature. In the present analysis, the temperature of specimens has been determined with various types of gases (helium/ argon/ helium-argon mixture) filled in the compartment. Using the calculation methodology and simulation analysis the appropriate He-Ar gas mixture can be selected to obtain a desired irradiation temperature in the specimens.Establishment of high temperature nicrobrazing procedure and qualification of brazed joints have been carried out. Fabrication of instrumented capsules requires the development of thin-walled joints capable of withstanding high temperatures. High-temperature brazing method has an advantage of joining multiple metal-sheathed cables such as thermocouples through a solid stainless steel plug in a single operation. High-temperature nicrobrazed joints under argon atmosphere have been produced as part of the project work. An induction heating technique has been used for this development. Protective atmosphere is required for high-temperature brazing to prevent oxidation of the base metal and the filler metal during the brazing operation. Commercial argon gas (99.996% pure) has been used and brazed joints have been developed. Brazing procedure has been established and development of high temperature nicrobrazed joints using induction heating in an argon gas environment has been done. Helium leak, metallographic, micro hardness tests, and sodium compatibility test have been carried out on the brazed samples. Comparative study was carried out on weld joints developed by high temperature nicrobrazing, laser and GTAW joining processes. During assembly of an irradiation capsule, requires a weld joints at tube to end plugs. For this we need to optimize the parameters of available joining methods to qualify the tests according to the standards. Helium leak test, Metallographic

and Micro hardness tests have been carried out on the joints made by laser, GTAW and high temperature nicrobrazing joining processes.

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2. "Development of out-of-pile version of instrumented irradiation capsule for determination of online creep deformation", Sadu Venkatesu, Rajesh Saxena, M. Muthuganesh, P. K. Chaurasia, S. Murugan and S. Venugopal, Springer Transactions of the Indian Institute of Metals, Vol.69 (2), 283-287, 2016, *DOI: 10.1007/s12666-015-0808-1.*
3. "Development of High-temperature Nicrobrazed joints using Induction Heating in an Argon gas Environment", Sadu Venkatesu, P.K.Chaurasia, S.Murugan and S.Venugopal, Springer Transactions of the Indian Institute of Metals, 2015, *DOI 10.1007/s12666-015-0696-4*.
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2. "Development of High-Temperature brazed joints and its Compatibility test with High Temperature Sodium", P.K. Chaurasia, K. Chandran, Sadu Venkatesu, S. Murugan, S. Anthonysamy, S. Venugopal and T. Jayakumar, Presented in National Welding Seminar at Jamshedpur , Jan 22- 24, 2015.
3. "Design and Analysis of Instrumented Irradiation Capsule for Online Determination of Uniaxial Creep behavior in Structural specimen", Sadu Venkatesu, K.A. Gopal, M. Muthuganesh, R. Saxena, S. Murugan, S. Venugopal and T. Jayakumar, Presented in International Symposium for Research Scholars at IIT Madras, Dec 11-13, 2014.
4. "Development of High-temperature Nicrobrazed joints using Induction Heating in an Argon gas Environment", Sadu Venkatesu, P. K.Chaurasia, S.Murugan, S.Venugopal and T. Jayakumar, Presented in National Weld Meet at Mohammed Satak College of Engineering, Keelankarai, Sep 02-03, 2014.
5. "Determination of Temperature of Structural Material Specimens in an Irradiation Capsule", Sadu.Venkatesu, S. Murugan and S.Venugopal, Presented in 5th International Symposium for Research Scholars at IIT Madras, Dec 13-15, 2012.

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107. Name : **Ali Ajmi**
Enrolment No. : PHYS01201204001
Date of Award of degree : 07.10.16
Constituent Institute : Bhabha Atomic Research Centre
Title : A Study Of Muonless Events And An Attempt To Improve The Hierarchy Sensitivity Through Neural Networks At Ical@Ino.

Abstract

The Iron-CALorimeter or the ICAL is the main detector to be set up at INO (India-based Neutrino Observatory). It is a giant magnetized neutrino detector for studying the atmospheric neutrino interactions. The present study is based on the ICAL detector, and deals with the atmospheric neutrinos. This enables us to study the oscillation phenomenon of the neutrinos, the added advantage being the fact that we can study the atmospheric neutrinos travelling through the earth.

This research work includes the study of both the kinds of the atmospheric neutrino events to be seen in the ICAL detector: the shower-like events or the muonless neutrino events and also the muon-track-containing neutrino events. High energy electron neutrino or antineutrino interactions have been studied only in IMB, Kamiokande and Super-Kamiokande before. INO gives us another chance to study them in detail. We propose a method to extract the atmospheric electron neutrino (antineutrino) data from the ICAL data. We also studied the muon neutrino charged current interactions, and attempted to improve the hierarchy sensitivity of the ICAL, which is its primary objective, by applying the neural network analysis. We also showed that the use of neural network cancels the effects of the background due to other neutrino interactions. Even after including the systematic uncertainties, ICAL can still achieve a 3-sigma sensitivity in its main goal.Apart from the above studies, this research also involves the technical skills of incorporating multiple new options in the Monte Carlo neutrino event generator called the GENIE.

Publications

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Other Papers:

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2. mproving the hierarchy sensitivity of ICAL using neural network by Ali Ajmi, Abhish Dev, Mohd. Nizam, Nitish Nayak, S.Uma Sankar: arXiv:1510.02350.

Conference Presentations :

1. Oral Presentation on Energy and Direction Estimation of neutrinos in muonless events at ICAL by Ali Ajmi and S. Uma Sankar: Proceedings published in Springer Proceedings in Physics, XXI DAE-BRNS High Energy Physics Symposium Proceedings, Guwahati, India, December 8 # 12, 2014 Editors: Bhuyan, Bipul (Ed.).
2. Poster Presentation on Inclusion of GENIE as ν -Event Generator for INO by Ali Ajmi and Gobinda Majumder @ XXI DAE-BRNS High Energy Physics Symposium, Guwahati, India, December 8 # 12, 2014.

3. Poster Presentation on Muonless Events in ICAL @ INO by Ali Ajmi and S. Uma Sankar @ EPS-HEP Conference Vienna, Austria, 22-29 July, 2015: Proceedings published in PoS (Proceedings of Science) EPS-HEP2015 (2015) 045, SISSA (2015-10-04).
4. Oral Presentation on Study of Muonless Events in ICAL @ INO by Ali Ajmi and S. Uma Sankar @ NSPDI-15, IICHEP, Madurai, India, 27-31 March, 2015.
5. Poster Presentation on Muonless Events in ICAL @ INO by Ali Ajmi and S. Uma Sankar @NNN15, Stony Brook University, New York, 28-31 October 2015.

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108. Name : **Sumit**
Enrolment No. : PHYS01201104020
Date of Award of degree : 07.10.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Nanoparticle Effect On Structural Evolution Of Protein-Surfactant Solutions.

Abstract

Nanoparticles, proteins and surfactants are three major components in soft condensed matter. Each one of these is extensively used for specific applications. Further, many additional applications arise by adjoining these components together to obtain interesting functional objects. The present thesis provides an understanding of the complex structures in these multi-component systems. The charged silica nanoparticles, BSA protein and three different surfactants (SDS, DTAB and C12E10) have been used as model systems. The systems are characterized by scattering techniques SANS and DLS. In particular, SANS with easy possibility to vary the contrast has been utilized to study such multi-component systems. The protein-surfactant systems under varying solution conditions have been investigated. In particular, the structure and interaction of BSA protein with ionic (anionic SDS and cationic DTAB) and nonionic C12E10 surfactants are found to very different. The ionic surfactants strongly bind to the protein and form bead-necklace structure, whereas protein does not show any change with the nonionic surfactant. In each of these surfactants, silica nanoparticle effect on protein-surfactant systems has been examined. The surfactant-dependent different microstructures of nanoparticle aggregates (mass and surface fractals) are formed along with enhanced protein-surfactant interactions in the resultant nanoparticle-protein-surfactant systems. The interactions in these systems are governed by the competition of electrostatic (repulsive and/or attractive) and attractive depletion interaction.

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2. Cationic versus Anionic Surfactant in Tuning the Structure and Interaction of Nanoparticle, Protein, and Surfactant Complexes Sumit Mehan, V. K. Aswal and J. KohlbrecherLangmuir 30, 9941 (2014).
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4. Structure and Interaction of Silica Nanoparticle, BSA Protein and Mixed Nonionic-Ionic Surfactant ComplexesSumit Mehan, V. K. Aswal and J. KohlbrecherPhys. Rev. E (Submitted).
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11. Role of Electrostatic Interaction on Surfactant Induced Protein UnfoldingSumit Mehan, S. Kumar and V.K. Aswal AIP Conf. Proc. 1512, 160 (2013).
12. Probing Structures of Multi-components Systems comprising Protein, Surfactant and Nanoparticle in Aqueous SolutionSumit Mehan, S. Kumar, V. K. Aswal and R. SchweinsInternational Symposium on Neutron Scattering, BARC, Mumbai (2013).
13. Observation of Adsorption vs. Depletion Interaction in Nanoparticle-Protein SystemSumit Mehan, S. Kumar and V.K. AswalInterdisciplinary Symposium on Material Chemistry, BARC, Mumbai (2012).

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109. Name : **Saikat Bhattacharya**
Enrolment No. : LIFE09201004024
Date of Award of degree : 14.10.16
Constituent Institute : Tata Memorial Centre
Title : Chromatin Organisation: Molecular Role of H2A Variants.

Abstract

Histones are a class of highly conserved basic proteins and packaging the genome was the primary function previously attributed to them. The core histones comprise of H2A, H2B, H3 and H4 which assemble as hetero-oligomers toform the octameric protein core of the fundamental repeating unit of chromatin, the nucleosome.Histone genes are presentin clusters and in multiple copies. For instance, in humans, H2A is coded by 16 genes. All of these genes do not code for the identical protein and give rise to sequence divergent forms of histones termed isoforms. H2A isoforms are known to exhibit altered expression under different physiological conditions. Their distinct functional effects remain a matter of investigation and the mechanistic basis of the non-redundancy is elusive.Here, we show isoform H2A.1 exhibits drastically altered

expression pattern in normal tissues and cancer cells. It is of functional importance as H2A.1 promotes cell proliferation in a context dependent manner. For carrying out comparative analysis of the stability of H2A.1 and H2A.2 containing nucleosome and sub-nucleosomal complexes *in vitro*, the histone proteins were recombinantly purified. Further, sub-nucleosomal complexes were reconstituted and purified. Biophysical characterization shows that M51L alteration at the dimer interface decreases the temperature of melting of H2A.1-H2B by ~3 ^{0}C as compared to H2A.2-H2B dimer. Further, M51L and K99R substitutions makes H2A.1 containing nucleosomes more stable by increasing the number of hydrogen bonds and hydrophobic interactions. Interestingly, the same two substitutions have the most prominent effect on cell proliferation, suggesting, that the nucleosome stability is intimately linked with the physiological effects observed.In summary, the incorporation of the histone isoform H2A.1 results in increased nucleosome stability, which is expected to contributeto the contextual alteration in global transcription pattern and other chromatin mediated processes.

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4. Carcinogenesis, ACTREC, Navi Mumbai, India, 2015.
5. The Asian Forum of Chromosome and Chromatin Biology, JNCASR, Bangalore, India, 2015.
6. 4th Asian Conference on Environmental Mutagens, IICB, Kolkata, India, 2014.
7. Biopaschim, ACTREC, Navi Mumbai, India, 2014.
8. Frontiers in Modern Biology, IISc, Bangalore, India, 2013.

110. Name : **Ram Avtar Jat**
Enrolment No. : CHEM01201004018
Date of Award of degree : 14.10.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Investigation of Effects of Ternary Alloying on the Hydrogen Storage Behavior of ZrCo Alloy.

Abstract

This thesis deals with the consolidated efforts to find a suitable ternary alloy for storage, supply and recovery of hydrogen isotopes. A systematic approach has been applied to investigate the effect of ternary alloying on the hydrogen isotope storage properties of ZrCo alloy. Alloys of composition $ZrCo_{1-x}Ni_x$ (x = 0.1, 0.2 and 0.3), $ZrCo_{0.9}Fe_{0.1}$ and $Zr_{1-x}Ti_xCo$ (x = 0.1, 0.2 and 0.3) were prepared and characterized. The hydrogen isotope storage behavior of Zr-Co-M ternary alloys was systematically investigated by generating the hydrogen/deuterium desorption pressure-composition isotherms (PCIs) by employing Sieverts' type apparatus. The thermodynamic parameters of the de-hydrogenation reactions and their corresponding isotopic effects were evaluated. Hydrogen induced disproportionation behavior of Zr-Co-M ternary alloys was investigated by hydrogen absorption-desorption cyclic life and isothermal studies. The phenomenon of hydrogen induced disproportionation in different Zr-Co-M ternary alloys was further investigated by employing neutron powder diffraction (NPD) technique. The extensive work carried out in this thesis enable to identify a suitable ternary substituent for effective storage, supply and recovery of hydrogen isotopes in particular tritium.This study reveals that, all alloys crystallize in b.c.c. type single cubic phase similar to ZrCo. A single desorption plateau is observed for all the pressure-composition isotherms (PCIs). The normal hydrogen isotope effect is observed for all ternary alloys which shows that equilibrium pressure of deuterium is higher than that of hydrogen at all experimental temperatures. Based on the structural studies, a modified crystal structure for $ZrCoD_3$ with occupancy of new interstitial site (8*e*) for deuterium atom was proposed. Systematic investigations on all ternary alloy deuterides establishes the effect of ternary alloying on the occupancy of new 8*e* site and Zr-D distance. Considering the PCT studies, hydrogen induced disproportionation studies and structural studies, it is proposed that among the alloy studied, $Zr_{0.8}Ti_{0.2}Co$ alloy is the best suitable non-pyrophoric and non-radioactive ternary alloy as a substitute for the conventionally used highly pyrophoric uranium bed for tritium storage applications. This alloy has potential for its use in tritium handling facilities for storage, supply and recovery of hydrogen isotopes.

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6. "Synthesis, characterization and hydrogen isotope storage properties of Zr-Ti-Co ternary alloys", Ram Avtar Jat, Subhasis Pati, S.C. Parida, Renu Agarwal and S.K. Mukerjee, Communicated to *International Journal of hydrogen energy* (MS # HE-D-16-01607).
7. "An analogy of interstitial site occupancy and hydrogen induced disproportionation of $Zr_{1-x}Ti_xCo$ ternary alloys", Ram Avtar Jat, Ripandeep Singh, Subhasis Pati, P.U. Sastry, A. Das, Renu Agarwal and S.C. Parida, Communicated to *The Journal of Physical Chemistry C* (MS # jp-2016-08700e).

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1. Hydrogen isotope storage behavior of $Zr_{1-x}Ti_xCo$ alloys, Ram Avtar Jat, Subhasis Pati, S.C. Parida, Renu Agarwal, S.K. Mukerjee, 20th DAE-BRNS International Symposium & Workshop on Thermal Analysis, THERMANS-2016, January 18-20, 2016, Indian Institute of Technology (BHU) Varanasi, Varanasi, India, pp. 77.
2. Hydrogen induced disproportionation studies on Zr-Co-M (M=Ni, Fe, Ti) ternary alloys, Ram Avtar Jat, Subhasis Pati, P. U. Sastry, V.B. Jayakrishnan, S.C. Parida, Renu Agarwal, S.K. Mukerjee, 20th DAE-BRNS International Symposium & Workshop on Thermal Analysis, THERMANS-2016, January 18-20, 2016, Indian Institute of Technology (BHU) Varanasi, Varanasi, India, pp. 78.
3. Effect of Ni content on hydrogen occupancy in $ZrCo_{1-x}Ni_x$ deuterides, Ram Avtar Jat, Ripandeep Singh, S.C. Parida, A. Das, Renu Agarwal, A.R. Joshi, K.L. Ramakumar, 58th DAE-Solid State Physics Symposium (DAE-SSPS-2013), December 17-21, 2013, Thapar University, Patiala, Punjab.
4. Hydrogen isotope storage behavior of $ZrCo_{1-x}Ni_x$ alloys, Ram Avtar Jat, S.C. Parida, Renu Agarwal, A.R. Joshi and K.L. Ramakumar, 19th DAE-BRNS International Symposium & Workshop on Thermal Analysis, THERMANS-2013, December 19-21, 2013, Bhabha Atomic Research Centre, Mumbai, India, pp. 141.
5. Hydrogen storage behavior of $ZrCo_{1-x}Ni_x$ alloys, Ram Avtar Jat, S.C. Parida, Renu Agarwal, S.G. Kulkarni, DAE-BRNS 4th Interdisciplinary Symposium on Materials Chemistry (ISMC), December 11-15, 2012, Bhabha Atomic Research Centre, Mumbai, India, pp. 150-151.
6. Hydrogen sorption-desorption studies on ZrCo-Hydrogen system, Ram Avtar Jat, S.C. Parida, Renu Agarwal and S.G. Kulkarni, 18th DAE-BRNS International Symposium & Workshop on Thermal Analysis, THERMANS-2012, January 31-Feburary 4, 2012, Bhabha Atomic Research Centre, Mumbai, India, pp. 350.

111. Name : **Neetika**
Enrolment No. : PHYS01201004020
Date of Award of degree : 14.10.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Nature Of Magnetic Ordering In Doped Hexagonal And Orthorhombic Manganites

Abstract

In the present work the effect of substituting with magnetic and non magnetic ions, at the A- and B-site, on the magnetic properties, electronic properties and variation in crystal structure of hexagonal $YMnO_3$ and orthorhombic $CaMnO_3$ have been investigated. $YMnO_3$ is a hexagonal frustrated antiferromagnetic system with T_N~ 75K. Below the T_N, anomalies in the volume and dielectric behavior are observed indicating magnetoelastic and magnetoelectric coupling, respectively. The role of the magnetic structure on the frustration behavior and physical properties has been studied in this compound. Toward, this study, perturbation in the form of doping at the Y- and Mn-site has been carried out. The layered triangular arrangement of the spins leading to frustration are significantly altered on partially substituting Y by magnetic ions viz., Yb, Er, Ho, and Tb. Thereby lowering the frustration in these compounds. This behavior is attributed to the additional interaction between R and Mn which in turn alters the Mn-Mn interactions. In the case of doping by Ti^{4+} (d^0), Fe^{3+} (d^5) and Ga^{3+} (d^{10}) at Mn-site the magnetic structure display significant differences between the three dopants. Large dielectric anomalies are observed coinciding with the T_N in these compounds which we show to scale with sub lattice magnetization obtained from neutron diffraction and follows a M^2 behavior close to T_N in agreement with predictions of Landau theory.$CaMnO_3$ has a G-type AFM structure (T_N ~125 K) with an additional weak ferromagnetic component in its ground state. Electron doping studies at Ca- and Mn-site substitution leads to different magnetic ground state. Doping in the $CaMnO_3$ leads to the presence of mixed valent Mn ions, which is responsible for the different electronic and magnetic properties. We have found phase separated magnetic ground state for $Ca_{1-x}Y_xMnO_3$. We find that as against Ca-site doping, the Mn site substitution ($CaMn_{1-x}Fe_xO_{3-\delta}$) favors canted G-type structure. The debate over phase separation versus canted magnetic structure continues to be of interest in electron doped (Mn^{4+} rich) compounds.

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3. Magnetic Structure Of Multiferroic Manganites, $YMn_{1-x}M_xO_3$ (M = Ga, Ti; x = 0, 0.1) NeetikaSharma and A. Das International Symposium on Neutron Scattering 2 39 (2013).
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5. Effect of Fe doping on the Structural, Magnetic, and Dielectric Properties of $YMnO_3$ Neetika, A. Das, S. K. Mishra, C. L. Prajapat DAE Solid State Physics Symposium 58 239 (2013).
6. Phase separated behavior in Yttrium doped $CaMnO_3$ Neetika Sharma, A. Das, Amit Kumar, C. L. Prajapat, , and M. R. Singh 5th Conference on Neutron Scattering 5 49 (2015).

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112. Name : **Subhankar Manna**
Enrolment No. : ENGG01200904022
Date of Award of degree : 21.10.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Studies In Reactive Precipitation: Morphology Of Ammonium Diuranate.

Abstract

Ammonium diuranate (ADU) is one of most important intermediate products in nuclear industries. Production processes and properties of uranium oxide used as fuel in power reactors and uranium metal used as fuel in research reactors largely depend on ADU characteristics. ADU is generally produced by reactive precipitation process where uranyl solution (either nitrate or fluoride) reacts with ammonia. ADU reaction is very fast and product is sparingly soluble. This causes very high degree of supersaturation. The involved mechanisms of nucleation, growth, aggregation and breakage occur simultaneously. These kinetic parameters (nucleation, growth, agglomeration and breakage) in turn have an effect on the particle size distribution and morphology. ADU is first intermediate product in solid powder form in flow sheet of uranium metal or uranium oxide production. Properties of subsequent intermediate products are inherited from ADU. Morphology of ADU powders controls their flow-ability, surface area, carryover losses and tap density. The most significant factors affecting the kinetic parameters are degree of supersaturation, flow field pattern, mixing, residence time and process parameters like temperature, concentration etc.Platelet morphology of ADU has been observed using scanning electron microscopy (SEM). ADU basically consists of primary platelets. These primary platelets form primary agglomerates. These agglomerates are also connected with each other to form secondary agglomerates. ADU particles of larger platelets and high surface area due to porosity are favourable. Over all rounded shape is also helpful to increase flow-ability. In the present work, an effort has been given to study the effects of uranium concentration, temperature, impeller type and impeller speed on the morphology and the other properties of ADU. It has been observed that growth of platelets and surface area increases with an increase in the uranium concentration, temperature, the impeller power number and rotational speed. But effect of temperature has been found to be more dominant. Temperature, type of impeller and impeller speed are optimized as 50 °C, PBT and 500 RPM respectively based on the studies on precipitation from nitrate solution.ADU produced by reaction of uranyl nitrate solution and gaseous ammonia has calcined in a muffle furnace at different temperature to study effect of calcination temperature on morphology and physical properties of calcined product of ADU (uranium tri oxide). The progress of the precipitation reaction via both the nitrate and fluoride route is monitored through measurement of pH and concentration of soluble uranium and composition of ADU. XRD pattern shows that the ADU produced from uranyl nitrate solution (UNS) consists of orthorhombic $3UO_3.NH_3.5H_2O$ and hexagonal $2UO_3.\ NH_3.\ 3H_2O$. On contrast, the ADU produced from uranyl fluoride solution (UFS) consists of orthorhombic $(NH_4)_3UO_2F_5$, hexagonal $(NH_4).(UO_2)_2F_5.4H_2O$ and hexagonal $2UO_3.NH_3.3H_2O$ with dominancy of $2UO_3.NH_3.3H_2O$. ADU produced from both the UNS and the UFS has calcined to UO_3, further reduced to UO_2 and hydroflorinated to UF_4 at similar condition. Both chemical and

physical properties of the products are systematically analyzed to understand how properties of UF_4 are inherited from its precursors. It has been observed that reduction of UO_3 to UO_2 is lesser in UFS route than UNS route due to presence of fluoride in ADU and subsequent UO_3.This causes more presence of UO_2F_2 in UF_4 produced via UFS route. Surface area of UO_2 obtained from UFS is lesser than that of UNS route. This is why UF_4 produced via UFS route content more AOI than UF_4 produced via UNS route. UO_3 via nitrate route consists of orthorhombic UO_3 and orthorhombic U_3O_8 and UO_3 via UFS route consists of hexagonal UO_3 and hexagonal U_3O_8. Crystal phase analysis shows that, inspite of different compositions of ADU produced by the two routes, crystal structure of UO_2 and UF_4 produced by two different routes are similar.

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3. "Study on particle morphology during ammonium diuranate precipitation", S. Manna, P. U. Sastry, S. V. Kadam, S. K. Satpati, S. B. Roy and J. B. Joshi, DAE-BRNS 4th Interdisciplinary Symposium on Materials Chemistry 2012, BARC, Mumbai. December 11-15, 2012

113. Name : **Anirban De**
Enrolment No. : ENGG04200804001
Date of Award of degree : 21.10.16
Constituent Institute : Variable Energy Cyclotron Centre
Title : A Novel scheme for DSP based Power Converter Control.

Abstract

The aim of the research is to devise a novel scheme for DSP based power converter coupled to a Superconducting Magnetic Energy Storage (SMES) system to mitigate voltage sags originating in the utility mains so as to keep the load voltage free of any interruptions.The power quality is one of the most important issues in the power distribution system. Many critical machines or industrial processes, especially those controlled by computers, are sensitive to voltage sag or short interruptions in supply. These disturbances increase the down time of the machine or process and hence the cost of production. SMES is a clean environment-friendly attractive solution for the power quality problems which can mitigate short time voltage fluctuation and sag. The associated control philosophy is based on correctly identifying the voltage sag in the AC utility lines and efficiently compensating it, both in amplitude and phase, by appropriately switching the power devices.Based on the schemes elaborated in literatures, the Flexible AC Transmission System (FACTS) type controllers were introduced and their applicability discussed. A technical comparison was made based on which the selection of the proposed series scheme viz., Dynamic Voltage Restorer (DVR), was justified. Further, the switching scheme of the central power device i.e., the Voltage Source Inverter (VSI) was elaborated and arguments for its applicability as regards to efficient DC bus utilization and voltage sag identification were reviewed.A digital control system was designed for the VSI that utilized a Software Phase Locked Loop (SPLL) for phase locking and voltage sag detection. The need of a prefilter to bandlimit the input signal and the requirement for the controller loop filter to eliminate the inherent double frequency component were indicated. The SPLL was designed to incorporate a bandpass prefilter for allowing only the preferred frequency in the system. The loop filter employed a bandstop filter cascaded to a PI controller to selectively eliminate the high frequency component and the steady-state error simultaneously. The analog design was translated to its bilinear transformed discrete equivalent and stability was checked theoretically. Difference equations were derived from the discrete model. A fixed point DSP based controller was programmed to implement the same. It was utilized for online phase locking, sag computations and Space Vector Pulse Width Modulation (SVPWM) based switching generator for the inverter bridge besides handshaking signals between the subsystems of the integrated DVR.A novel scheme of low pass filter system for the VSI was presented. A set of performance indices was defined reflecting the quality of the filter and also the ratings of the filter components. An additional energy function based performance index for the inductor of the filter system was also put forward. It thus considered both the attenuation and the practicability of implementation of the filter system as regards the volume and availability of components. The way to utilize transformer turns-ratio advantageously was indicated in the final scheme. In the process, an attenuation of 60 dB was achieved at the switching frequency. The design was implemented in actual hardware. Tests were carried out configuring it both as a standalone inverter and a VSI employed in DVR. The test results corroborated the design values. The design was kept generalized so that it may be applied on any VSI system. Detailed analysis of the model for a balanced 3- system was also presented that decoupled it for 1- analysis.The VSI was configured for SMES based DVR for a 3- 240 V, 50 Hz, 3.45 kW load for voltage sag mitigation according to IEEE 1159-1995. Voltage sags of varying depths were mitigated for 40 ms to 6 sec with phase locking. This demonstrated the system's performance for satisfactory phase locking and voltage compensations for momentary sags and partly for instantaneous and temporary sags.

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1. Anirban De, U. Bhunia, S. Bandopadhayay, J. Pradhan, Subimal Saha, "Design, development and testing of a 0.6MJ/3.4kW Prototype Superconducting Magnetic Energy Storage System based Dynamic Voltage Restorer", 26th International Cryogenic Engineering Conference International Cryogenic Materials Conference (ICEC 26 - ICMC 2016), Manekshaw Centre, New Delhi, India, Mar 7-11, 2016.
2. Anirban De, Santwana Kumari, V.K. Khare, S.S. Pal, Anindya Sadhukhan, V.K. Meshram, S.K. Thakur, Subimal Saha, "Design, Development and Testing of a DSP based Dynamic Voltage Restorer" , Proceeding of the 3rd International Symposium on Electronic System Design (ISED2012), BESU, Shibpur, Howrah, Dec 19-22, 2012.

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114. Name : **Abhishek Chowdhury**
Enrolment No. : PHYS08200905004
Date of Award of degree : 25.10.16
Constituent Institute : Harish-Chandra Research Institute
Title : Finer Consistency Checks On Bps Black Hole Entropy In String. Theory.

Abstract

The primary research presented in this thesis revolves around the central theme of black hole entropy matching, widening its scope and applicability to further reinforce the internal consistency of string theory. Black holes have an effective classical description in supergravity which in itself is the low energy theory from string theory. On the other hand, black holes have a quantum description in terms of D-branes and strings fluctuating on these branes. The microstates originating from string fluctuation should make up for the entropy of the black hole. For a large class of SUSY black holes in N=4 & N=8 theories the leading order answers match but our focus throughout would be to illustrate such matching in next to leading order. Listed below are the major results of the such studie

- We attempted to give a physical explanation behind a set of ad hoc rules necessary to match the microscopic counting to the entropy of quarter-BPS black holes in N = 4 string theory.
- We precisely reproduced certain logarithmic terms emerging from the large charge expansion of twisted microscopic indices from respective quantum corrections to quarter-BPS & one eight-BPS black holes in N = 4 & N = 8 supergravity theories.

Publications

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1. Do all BPS Black Hole Microstates Carry Zero Angular Momentum? Abhishek Chowdhury, Richard S. Garavuso, Swapnamay Mandal, Ashoke Sen. JHEP 1604 (2016) 082 DOI: 10.1007/JHEP04(2016)082
2. BPS State Counting in N=8 Supersymmetric String Theory for Pure D-braneConfigurations. Abhishek Chowdhury, Richard S. Garavuso, Swapnamay Mandal, Ashoke Sen. JHEP 1410 (2014) 186 DOI: 10.1007/JHEP10(2014)186
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115. Name : **Avinanda Chaudhuri**
Enrolment No. : PHYS08201004006
Date of Award of degree : 25.10.16
Constituent Institute : Harish-Chandra Research Institute
Title : Seesaw And Seesaw-Like Scenarios: Some Phenomenological Implications.

Abstract

The Standard Model (SM) of particle physics has been extremely successful in describing most of the observed phenomena in particle physics. However, there is a strong motivation for physics beyond the SM, to address some yet unexplained observations, which include, small masses and mixing pattern of neutrinos, existence of Dark Matter (DM) and Dark energy in the Universe, matter-antimatter asymmetry of Universe and so on. Also, in the Large Hadron Collider (LHC) era, we hope to test the theory beyond the SM, which describes physics at the TeV scale. So, physics beyond the SM is a serious study for any aspiring physicist.In the first part of the thesis, phenomenology of doubly-charged scalar decays in Type II seesaw framework and usefulness of these decays at the LHC has been described. We have shown that, when a doubly-charged scalar decays into a singly-charged scalar plus a W boson of same sign, then this decay really dominates over all other decays, by taking all the vevs and coefficients of Lagrangian to be real. We have also pointed out the distinction between having a single triplet and two triplets in the scenario, at the LHC, by defining ratios of events emerging from two, three and four-lepton final states with missing transverse energy(MET). We found that, after applying suitable cuts to suppress the SM background, these ratios are widely different in two-triplet case as compared to single-triplet model --- this provides a way to distinguish between the two scenarios at the LHC. To see the phenomenology including CP-violation, we made a minimal extension of the simplified scenario by postulating one CP-violating phase to exist. We observed that the heavier doubly-charged scalar decays dominantly into lighter doubly-charged scalar plus SM Higgs. This, in turn, opens up a spectacular signal at LHC, especially when the lighter doubly-charged scalar mostly decays into two same sign leptons, leading to the decay of heavier doubly-charged scalar into a pair of same-sign leptons plus SM Higgs. We pointed out some rather interesting effect of presence of phase. If the mass differences do not allow the above mentioned decays when the phase is absent, they eventually open-up with the increase in phase of triplet vev, when all other parameters are at fixed values. Another notable effect of presence of phase is that, the contribution of triplet vev to neutrino masses gets suppressed. This results in an increase in

corresponding Yukawa couplings. This is reflected in the fact that, the decay of a doubly-charged scalar into two same-sign leptons too has non-negligible branching ratios.In the second part of the thesis, we proposed an extension of the type-III seesaw model for neutrino masses. We proposed two Z2-odd fermion fields: a Y=0 triplet and a neutral singlet that appears as a heavy sterile neutrino. The lightest Z2-odd fermionic state emerges as the DM candidate in this work. The requisite rate of annihilation is ensured by postulating some Z2 preserving dimension-five operators. We got a large region of parameter space that satisfies the correct relic density requirement and the bound imposed by XENON 100 and LUX data on WIMP-nucleon cross section in both the cases of self-annihilation and co-annihilation of DM candidate.

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1. "Texture zeros and type II seesaw mechanism",A. Chaudhuri,Nu Horizon, Harish-Chandra Research Institute, Allahabad, 17-19 th March, 2016.

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116. Name : **Vidya Sagar Yellapu**
Enrolment No. : ENGG01201104006
Date of Award of degree : 25.10.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Data Reconciliation Based Scheme For Sensor Fault Detection.

Abstract

In controlled systems, two kinds of errors that commonly arise in the measurement signals are random errors and gross errors or faults. These errors invalidate the signals of potential interest used for feedback control, protection and estimation. Random errors are due to slight variations in operating conditions of the components and other probabilistic phenomenon. They cannot be completely eliminated but their effects can be reduced considerably with the use of filtering techniques and their statistical properties. On the other hand, faults are unpermitted deviations in one or more of the characteristic properties of the components from the acceptable, usual and standard conditions. Faults in system or process components including sensors, if not detected and diagnosed, establish the need for maintenance activities, endanger the system reliability, activate safety systems, cause operational upsets and reduce safety margins. A system that automatically nullifies the effects of these two kinds of errors is highly desirable. A measurement data-based Data Reconciliation (DR) scheme can be realized, which utilizes the algebraic relationships among the variables as redundant information to filter out the random errors. This scheme can also detect and eliminate faults from the signals, when it is coupled with a suitable Fault Detection and Diagnosis (FDD)

system. For sensor fault detection, this DR based FDD scheme is suitable as it doesn't need the dynamic model of the system, whose development is not only complex but also possibly erroneous.

FDD in nuclear reactors is a more crucial task, since they have stringent requirements for safety and economy. The instantaneous value of the thermal power generated in the reactor can be estimated from neutron flux. In large nuclear reactors, *e.g.* Advanced Heavy Water Reactor (AHWR), a large number of neutron flux detectors are placed both inside and outside the core for measurement of core flux. The neutron flux detectors might often be contaminated with the random errors and faults. In addition, the measurement signals from these detectors are of delayed nature because of their inherent dynamics. However, the delayed nature is tolerated when a compensation scheme is available.In AHWR, ion chambers and Vanadium Self Powered Neutron Detectors (VSPNDs) are respectively used for the in-core and ex-core detector applications. In this thesis, FDD of these detectors is attempted by tests such as Generalized Likelihood Ratio (GLR) method, Iterative Measurement Test and Iterative Principal Component Test, when used alongwith DR scheme, which includes detection, isolation and estimation of faulty signals. Firstly, the signals of ion chambers and VSPNDs are simulated using the mathematical model of the reactor, under typical operating transients of the reactor. Then, data driven methods such as Principal Component Analysis (PCA) and Iterative Principal Component Analysis (IPCA) are used for the development of the constraint model required for the DR based FDD scheme. The effectiveness of the scheme has been established through simulations performed on all the ion chambers and individual clusters of VSPNDs with consistent correlation patterns. For the FDD of VSPNDs, a model based scheme is also proposed in which the Kalman filter framework, a classical random error reduction technique, has been extended such that it also performs FDD using GLR method. This scheme dynamically compensates the detector signals for promptness; minimizes the random errors through Kalman filter; and performs FDD with GLR method. The implementation of this scheme has also been elaborated.

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117. Name : **Varchaswi K S Kashyap**
Enrolment No. : PHYS01201004018
Date of Award of degree : 25.10.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Studies on Resistive Plate Chambers (RPC) for INO and scintillators for reactor antineutrino detection.

Abstract

Neutrinos oscillate from one flavor to the other as they propagate. This shows that they possess a very tiny but finite mass which according to the Standard Model of particle physics is zero. The determination of this mass and precision measurement of the oscillation parameters has long standing implications on our understanding of nature like the origin of the universe and the matter – antimatter asymmetry. Some data of neutrino experiments at short source to detector distances are in favor of the existence of a new flavor of neutrino called the sterile neutrino that does not have any kind of interaction except through gravitation and mixing. Also the prospect of using neutrino detectors at few tens of meters from reactors to monitor them remotely has generated a lot of interest around the world. Detectors used for reactor monitoring can double up for sterile neutrino search.The magnetized Iron CALorimeter (ICAL) is a proposed detector at the India-based Neutrino Observatory (INO) which will be setup under a mountain in the Theni district of Tamil Nadu, India. The aims of this detector are the precision measurement of the neutrino oscillation parameters and determination of the neutrino mass hierarchy using atmospheric neutrinos. Gaseous detectors called Resistive Plate Chambers (RPC) are the active elements of ICAL. RPCs are fast detectors with good position and excellent time resolution. It has also been proposed to setup a 1 ton plastic scintillator array called ISMRAN (India's Scintillator Matrix for Reactor Anti-Neutrino) at a distance of ~10 m from the 100 MW_{th} Dhruva research reactor at BARC for developing the technology of reactor monitoring and sterile neutrino search.The thesis has been divided into two parts. The first discusses studies done on RPCs for the INO and the second discusses simulations and background measurements for antineutrino detection in context of reactor monitoring and sterile neutrino search.**Part I:** A plastic scintillator based hodoscope was constructed for characterizing large area RPCs both for the RE4 (4th Rear End cap disk) upgrade of the Compact Muon Solenoid (CMS) experiment at CERN and R & D towards RPCs for INO and related experiments. Tests on RPCs (1 m x 1 m) with readouts made of G10 and polycarbonate honeycomb have been performed. RPC performance with different front-end electronics namely ANUSPARSH-II, III and HMC based preamplifiers developed by Electronics Division – BARC, has been compared. Consistent results have been obtained with good RPC efficiency (~95 %). Indian Bakelite RPC R & D has been initiated.**Part II:** Plastic and liquid scintillator geometries have been simulated and compared using GEANT4 Monte Carlo simulation package. Plastic scintillator based geometry appears to be suitable due to its modularity, safety and portability. Background measurements have been performed using various detectors: BGO (Bismuth Germanium Oxide) for gamma, LYBO (Lithium Yttrium Borate) for thermal neutrons and Liquid scintillators for fast neutrons with different shielding configurations. Correlated event measurements have also been done using plastic scintillator bars. Fast neutron measurements have been done using digitizer based acquisition system.

Publications

Journal

1. V. K. S. Kashyap, L. M. Pant, A. K. Mohanty, and V. M. Datar,Simulation results of Liquid and Plastic scintillator detectors for reactor antineutrino detection - A comparison, *Journal of Instrumentation*, 11(03):P03005, 2016.

Accepted

1. V. K. S. Kashyap, C. Yadav, S. T. Sehgal, R. Sehgal, R. G. Thomas, L. M. Pant,K. Mohanty, Plastic scintillator based hodoscope for characterization of large area RPCs, Accepted in *Pramana - J. Phys*.

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1. Monte Carlo simulation for estimation of trigger rate in Cosmic Hodoscope at NPD-BARC, V. K. S. Kashyap et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 57 (2012) 936.*
2. Avalanche mode operation of a Glass RPC with humid gas mixture, V. K. S. Kashyap et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 58 (2013) 870.*
3. Simulation and conceptual design of a detector for sterile neutrino search and remote reactor monitoring, V. K. S. Kashyap et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 58 (2013) 946.*
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6. Background measurements at the DHRUVA reactor site for feasibility studies towards antineutrino detection from reactors, V. K. S. Kashyap et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 59 (2014) 978.*
7. Liquid and plastic scintillator detectors for detecting antineutrinos from reactors –A GEANT4 simulation study, V. K. S. Kashyap et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 59 (2014) 944.*
8. G-10 read out panel 1 m x 1 m as an option for RPCs in INO, S. T. Sehgal et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 59 (2014) 922.*
9. Time distribution measurements of prompt-delay events at the Dhruva reactor for detection of antineutrinos, V. K. S. Kashyap et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 60 (2015) 924.*
10. Simulation of detector response for antineutrino induced events with a proto-type plastic detector array, S. P. Behera et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 60 (2015) 1032.*
11. Variation in thermal neutron flux at the anti-neutrino measurement site in the Dhruva reactor, A. K. Singh et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 60 (2015) 968.*
12. Development of large area (1 m x 2 m) bakelite gas-gaps in India for INO and related experiments, V. K. S. Kashyap et al, *Proceedings of the DAE-BRNS Symp. on Nucl. Phys. 60 (2015) 946.*

118. Name : **Mohit Pramod Sharma**
Enrolment No. : ENGG01201104005
Date of Award of degree : 27.10.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Investigation On The Flow Distribution Within The Rod Bundle Of Ahwr

Abstract

The Advanced Heavy Water Reactor (AHWR) is a vertical pressure tube type, heavy water moderated and boiling light water cooled natural circulation based reactor. The coolant flow distribution in single and two phase flow condition is very important for AHWR rod bundle to ensure its safety and performance. Single phase flow condition exists in reactor rod bundle during start-up condition and up to certain length of rod bundle when it is operating at full power. However, being a natural circulation BWR, transition from single phase to two phase flow condition occurs in reactor rod bundle with increase in power. Prediction of thermal margin of the reactor has necessitated the determination of inter-subchannel mixing of coolant amongst these subchannels. The inter-subchannel mixing consists of three independent phenomena; turbulent mixing, void drift and diversion cross flow.Of course, two phase turbulent mixing studies are not new especially for conventional BWRs. However it is important to assess the models developed so far for these reactors for their accuracy and applicability to AHWR condition. In this study, assessment of two phase turbulent mixing models applicable to BWRs has been performed against existing experimental data for various subchannel geometries of BWRs. It is found that there are large errors between predictions by the empirical models and measured experimental data. Even there are large differences in prediction among the models and experimental data of turbulent mixing rate from one subchannel array to another. This is because mixing phenomena are highly geometry and operating condition dependent. It may be noted that, the subchannel geometry of AHWR rod bundle is completely different from conventional BWRs. The rods in AHWR bundle are arranged in circular subchannel array unlike conventional BWRs geometry in which rods are arranged in square-square, rectangular-rectangular and square-rectangular subchannel array. In the view of above, data obtained from conventional BWRs cannot be used for AHWR. In addition, AHWR being a natural circulation BWR, the effect of variation of mass flux in the subchannels on two phase mixing phenomena for AHWR specific geometry needs to be investigated. Since it is difficult to develop mechanistic model for different aspects of mixing (i.e. turbulent mixing, void drift and diversion cross flow) in the rod bundle, experiments were carried out in a scaled test facility of AHWR rod bundle. The facility simulates 1:1 geometry of 1/12th symmetrical section of AHWR rod bundle. Water and air was used as the working fluid and the inter-subchannel mixing tests were carried out. The turbulent mixing rate, void drift and diversion cross flow was experimentally measured for AHWR operating condition.Our results indicates that i. The turbulent mixing and void drift both are found to be dependent on void fraction and flow regimes even for low mass flux condition typical to AHWR geometry.ii. The magnitude of turbulent mixing rate due to turbulent mixing and diffusion coefficient due to void drift is found to be higher for AHWR subchannels geometry compared to conventional BWRs geometry for the same mass flux.iii. Also the magnitude of turbulent mixing rate and diffusion coefficient found to be increase with increase in superficial liquid velocity iv The cross flow resistance coefficient due to diversion cross flow in two phase flow is higher as compared to single phase flow.Empirical models were developed based on experimental data which could predict the inter-subchannel mixing due to turbulent mixing, void drift and cross flow quite accurately with an average error of ± 9 %. These models can be used to assess AHWR flow distribution and thermal margin.

Publications

Journal

1. Sharma, M.P., Nayak A.K., 2016. “Experimental investigation of two phase turbulent mixing rate under bubbly flow regime in simulated subchannels of a natural circulation pressure tube type BWR”. Experimental Thermal and Fluid Science (Elsevier), Vol. 76, Pages 228–237.
2. Sharma, M.P., Nayak A.K., 2015. “Determination of single phase turbulent mixing rate in simulated subchannels of a natural circulation pressure tube type BWR”. Nuclear Science and Engineering (ANS), Vol. 180, 175-185.
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6. Sharma, M.P., Nayak A.K., 2016. “Experimental investigation of void drift in simulated subchannels of a natural circulation pressure tube type BWR”. Paper submitted in Nuclear Technology (ANS). Accepted
7. Sharma, M.P., Nayak A.K., 2016. “Experimental investigation of diversion cross flow in simulated subchannels of a natural circulation pressure tube type BWR”. Nuclear Engineering and Radiation Science. (ASME).Communicated (Accepted with modification)

Conferences

1. Sharma, M.P., Nayak A.K., Kannan U. “Development of two phase turbulent mixing models for subchannel analysis relevant to BWR”. Proceedings of New Horizons in Nuclear Reactor Thermal Hydraulics and Safety, January 13-15, 2014, Mumbai, India.
2. Sharma, M.P., Nayak A.K., Kannan U. “Determination of single phase turbulent mixing rate in a simulated AHWR subchannels”. Proceedings of New Horizons in Nuclear Reactor Thermal Hydraulics and Safety, January 13-15, 2014, Mumbai, India.

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119. Name : **Sai Venkata Ramana A.**
Enrolment No. : PHYS01201104012
Date of Award of degree : 27.10.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Global renormalization group theoretic studies on liquid vapor phase transitions.

Abstract

Accurate prediction of the liquid-vapor phase transition and the critical point of materials continues to be an important topic of research in theoretical modeling of liquids. In this thesis a generalized version of global renormalization group theory (GRGT) for calculating Helmholtz free energy of a simple classical fluid is derived. The method improves upon mean-field Helmholtz free energy by including the effects of fluctuations using the Wilson's approach for functional integration without making the adhoc assumptions in earlier versions of GRGT. The generalized GRGT is applied to fluids with particles interacting with square-well and Lennard-Jones potentials. The new method produces flat isotherms in the two-phase region avoiding the unphysical Van-der Waals loop. Also, the liquid-vapor phase diagram(LVPD) is improved in the critical region. However, the LVPDs obtained for fluids with short range potentials have been found to be inaccurate. The reason for this disagreement is that the mean-field theory and the direct correlation function used in the calculation become inaccurate when the interaction potentials are short ranged. Combining the integral equation theory with the perturbation theory, a new mean-field method to evaluate the terms of perturbation series for Helmholtz free energy has been developed. The method, known as coupling parameter expansion(CPE) method, also allows for calculation of radial distribution function and direct correlation function. Seventh order version of the CPE method is applied to square-well and Lennard-Jones fluids and a significant improvement in obtained results over those of existing methods has been observed. Also it has been shown that the terms of CPE for radial distribution function and direct correlation functions scale with temperature for fluids with interaction potential having a hard core. Further improvement in the accuracy of LVPDs in the critical region has been attained by using the Helmholtz free energy and direct correlation function obtained from CPE method in the GRGT. A study of the scaling laws and the Yang-Yang anomaly in square-well fluids in the the critical region has been done using CPE+GRGT. The obtained critical exponents conformed to Ising universality class. The method could predict the Yang-Yang anomaly but the strength of anomaly differed from simulation. With the aim of applying CPE+GRGT to metals, a modified form of pair potential for metals has been proposed. The parameters of the potential for Aluminum, Copper, Potassium and Sodium have been obtained by fitting to the zero Kelvin isotherm. To determine the exact results given by the new potentials, we performed particle-transfer molecular dynamics simulations using the potentials and obtained the LVPDs of Aluminum, Copper, Potassium and Sodium. In the cases of Sodium and Potassium for which the experimental LVPDs are available, a significant improvement in the simulation results with new potentials has been observed over those of existing potentials. The CPE+GRGT has been applied to the potentials and a close agreement of our theoretical LVPDs with simulation data has been observed. Thus, in this thesis, an improved method for calculating the Helmholtz free energy of a fluid which takes into account the physics of liquid-vapor transitions in a more rigorous way has been developed. The method has been applied to model fluids and liquid metals modeled using empirical potentials with considerable success.

Publications

Journal

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2. A. S. V. Ramana, and S. V. G. Menon. "Coupling-parameter expansion in thermodynamic perturbation theory." Physical Review E 87.2 (2013): 022101.
3. A. S. V. Ramana, "Generalized coupling parameter expansion: Application to square well and Lennard-Jones fluids." The Journal of chemical physics 139.4 (2013): 044106.
4. A. S. V. Ramana, "On equivalence of high temperature series expansion and coupling parameter series expansion in thermodynamic perturbation theory of fluids." The Journal of Chemical Physics 140.15 (2014): 154106.
5. A. S. V. Ramana, "Molecular dynamics simulation of liquid–vapor phase diagrams of metals modeled using modified empirical pair potentials." Fluid Phase Equilibria 361 (2014): 181-187.
6. A. S. V. Ramana, "Application of renormalization group corrected coupling parameter expansion method to square well fluids." Physica A: Statistical Mechanics and its Applications 442 (2016), 137-148.

Other Publications :

1. A. S. V. Ramana, and S. V. G. Menon. "Application of the Englert–Schwinger model to the equation of state and the fullerene molecule." Physica A: Statistical Mechanics and its Applications 390.9 (2011): 1575-1584.
2. A. S. V. Ramana, "Molecular Dynamics Simulation of Liquid-Vapor Coexistence Curves of Metals." Journal of Physics: Conference Series. Vol. 377. No. 1. IOP Publishing, 2012.
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120. Name : **V. Prakash**
Enrolment No. : ENGG02200804006
Date of Award of degree : 3.11.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Ultrasonic technique for vibration measurement of immersed primary components in FBRs.

Abstract

This research work has been focused on vibration measurement of immersed components in the primary pool of FBRs. The main objective of the research is the development of ultrasonic technique for vibration measurement of immersed components in FBRs. Sodium is the coolant used in FBRs and is opaque to light. Coolant sodium and high temperature environment poses the challenges of direct vibration measurement techniques, hence calls for alternative solutions like ultrasonic techniques. Application of ultrasonic waves is investigated for its usefulness in measuring vibration of sodium-immersed components. Extensive studies were carried out and a measurement methodology was developed and optimized. All the challenging issues were successfully addressed and the end results were found to be very promising for applications in FBRs. Using the developed technique, measurements were carried out using simulated targets and a system named SONAR was developed for PFBR. As an extension to the project work, development of ultrasonic waveguide was also carried out. The wave guide is used for the measurement of vibration in hostile high temperature environment. The performance of the waveguide system was satisfactory and encouraging. The technique proved to be very promising for under sodium vibration measurements inside the reactor primary vessel without the use of high temperature sodium immersible ultrasonic sensors.Ultrasonic technique was studied and implemented for subassembly vibration measurement in PFBR and a measurement device (sonar) was developed for PFBR for subassembly vibration measurement during commissioning. Studies were also carried out for development of ultrasonic waveguide sensors for FBR applications. A waveguide system was developed and tested successfully and was also employed for vibration measurement of a target plate.

Publications

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2. V.Prakash, M.Thirumalai, M.Anandaraj, P.Anup Kumar, D.Ramadasu, G.K.Pandey, G.Padmakumar, C.Anandababu, and K.K.Rajan "Experimental qualification of subassembly design for Prototype Fast Breeder Reactor", Nuclear Engineering and Design 241 (2011) 3325–3332.
3. V.Prakash, P.Anup Kumar, M.Anadaraj, M.Thirumalai,C.Anandababu and K.K.Rajan "Flow induced vibration studies on PFBR control plug components", Nuclear Engineering and Design, Vol. 250, Sep 2012, pp. 725–734
4. V.Prakash, M.Thirumalai, R.Prabhakar and G.Vaidyanathan "Assessment of flow induced vibration in sodium-sodium heat exchanger, Nuclear Engineering and Design, Vol. 239, 2009, pp. 169-179.
5. P. Anup Kumar, R. Vidhyalakshmi, M. Thirumalai, S. Chandramouli and V. Prakash, "Development of SONAR device for fuel subassembly vibration measurement in PFBR", Journal of Acoustic Society of India, Vol 41, No. 3, 2014 (pp. 137-143).
6. R. Ramakrishna, P. Anup Kumar, M. Anandaraj, M. Thirumalai, V. Prakash, C. Anandbabu and P. Kalyanasundaram, NDE Technique for Reactor Core Vibration Measurement in FBRs, Journal of Non destructive Testing & Evaluation, Vol. 10, Issue 2 September 2011.
7. M. Thirumalai, M. Anandaraj, P. Anup Kumar, V. Prakash, C. Anandbabu, P. Kalyanasundaram, G. Vaidyanathan, Experimental investigation of weir instability in main vessel, Nuclear Engg. & Design, Volume 240 (2010), 84-91.

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1. P. Anup Kumar, R. Vidhyalakshmi, Sudheer Patri, S. Chandramouli, V. Prakash, et. al., Vibration measurements on PFBR fuel subassemblies, Int. Conf. VETOMAC X 2014, September 9-11, 2014, Manchester, UK.
2. P. Anup Kumar, R. Vidhyalakshmi, S. Chandramouli, V. Prakash, et. al., Development of SONAR device for fuel subassembly vibration measurement in PFBR, Acoustics 2013 Conference, New Delhi, India.
3. V.Prakash, P.Anup Kumar, M.Anandraj, M.Thirumalai, G.K.Pandey, Piyush Agarwal, Indranil banerjee, G.Padmakumar, C.Anadbabu, K.K.Rajan, Thermal hydraulics and FIV experiments simulating the reactor assembly of FBR, SMiRT Post conference Seminar on Fast Reactor Design, 14-15, November, 2011, Kalpakkam, India
4. R.Ramakrishna, P.Anup kumar, M.Anandraj, M.Thirumalai, V.Prakash, C.Anandababu and P.Kalyanasundram, NDE Technique for Core vibration measurement in FBRs, NDE 2010, Kolkata, India.
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121. Name : **Suman Rana**
Enrolment No. : CHEM01200904024
Date of Award of degree : 15.11.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Synthesis,Characterization And Biomedical Applications Of Surface Functionalized Nanoparticles.

Abstract

During the last decade, there has been extensive effort to explore applications ofnanostructured materials in various biomedical devices and processes. One of theprerequisite for successful use of nanoparticles for biological applications is its biocompatibility and ability to target to the site of interest. Interfacial modification of nanoparticles plays a crucial role in this respect. Magnetic nanoparticles offer a range of opportunities for biomedical research, as their response can be tailored by choosing from a variety of magnetic materials with different magnetic properties that can bemanipulated by the use of external magnetic fields and by modification of their surfaces with molecules specific for intended applications [1]. Magnetic nanoparticles are a major class of nanoscale materials with the potential to revolutionize current clinical diagnostic and therapeutic techniques. Due to their unique physical properties and ability to function at the cellular and molecular level of biological interactions, they are being actively investigated as the nextgeneration contrast agents for magnetic resonance imaging (MRI), carriers for targeted drug delivery, heating sources for hyperthermia treatment of cancer and magnetic separation agent in separation science [2-4]. The advantage of magnetic nanoparticles in biotechnology arises from a multitude of properties. First, they have sizes that place them at dimensions comparable to those of a virus (20–500 nm), protein (5–50 nm) or a gene (2 nm wide and 10–100 nm long). Second, the nanoparticles are magnetic, and hence can be manipulated by an external magnetic field gradient. Third and finally, nanoparticles have a large surface that can be properly modified to attach biological agents. Applications in nanobiotechnology impose strict requirements on the particles physical, chemical and pharmacological properties, including chemical composition, granulometric uniformity, crystal structure, magnetic behaviour, surface structure, solubility and low own toxicity. For example, in order for magnetic drug-targeting to be safe and effective (with the minimum amount of magnetic particles, a maximum of drug should be easily administered and transported to a specific site), the following parameters of thenanomagnets are critical: (a) particle size (small as possible to improve tissular diffusion, and to have long sedimentation times and high effective surface areas), (b) surface characteristics (easy encapsulation of the magnetic nanoparticles protects them from degradation and provides biocompatibility), and (c) good magnetic response. The recent surge of interest in nanotechnology has significantly expandedthe breadth and depth of magnetic nanoparticles research. They have been explored ina wide range of applications in the detection, diagnosis, and treatment of illnesses, such as cancer [5], cardiovascular disease [6], and neurological disease [7-8].Amongst the various magnetic nanoparticles, Fe_3O_4 nanoparticulates have received a great deal of attention due to their potential applications such as contrast agent for MRI, hyperthermia treatment of cancer and drug delivery. Surface modification of magnetic nanoparticles is important to render them notonly non-toxic, biocompatible, soluble in water, but chemically functional, and thus allow a targetable delivery with particle localization in a specific area [9]. Higher effective surface area of nanoparticles facilitates easy attachment of ligands, lower sedimentation rates (high stability in colloidal suspension) and improved tissular diffusion. For most of therapeutic applications, the first significant challenge is to avoid undesirable uptake of nanoparticles by the reticulo-endothelial system (RES) [10]. The next step is to achieve selective targeting of the system to the site of interest for the in-vivo studies. Surface functionalized small sized nanoparticles have higher diffusion rates which increase the concentration of nanoparticles at the centre of a blood vessel, thereby limiting the

interactions of nanoparticles with endothelial cells and prolonging the nanoparticles blood circulation time.The objectives of the present study have been the fabrication of surface modified Fe3O4 nanoparticulates, and the investigation of their structural/ microstructural, thermal and magnetic properties and exploration of their applications in biomedical field. The results obtained from the present investigations have been described and compiled under different chapters of this thesis, along with anintroduction to the topic. A brief account of each chapter has been given below.

Publications

Journal

1. “Folic acid conjugated Fe3O4 magnetic nanoparticles for targeted delivery ofdoxorubicin”,Suman Rana, N. G. Shetake, K. C. Barick,, B. N. Pandey, H. G. Salunke and P. A. Hassan *Dalton Trans.* (2016) accepted.
2. “PEG functionalized luminescent lipid particles for cellular imaging”Suman Rana, K. C. Barick, N. G. Shetake, G. Verma, V. K. Aswal, L. Panicker,B. N. Pandey and P. A. Hassan *Chem. Phys. Lett.* 2016, 659, 225-229.
3. “Stimuli responsive carboxyl PEGylated Fe3O4 nanoparticles for therapeutic applications” Suman Rana, K. C. Barick and P. A. Hassan *J. Nanofluids* 2015, 4, 1-7
4. “Surface modification of magnetic nanoparticles for therapeutic applications” K. C. Barick, Suman Rana and P. A. Hassan *J. Surface Sci. Technol.* 2015, 31, 123–132.
5. “Making sense of brownian motion: Colloids characterisation by dynamic light scattering” P. A. Hassan, Suman Rana and G. Verma *Langmuir* 2015, 31, 3-1
6. “Polyaniline shell cross-linked Fe3O4 magnetic nanoparticles for heat activated killing of cancer cells” Suman Rana, Neena V. Jadhav, K. C. Barick, B. N. Pandey and P. A. Hassan*Dalton Trans.* 2014, 43, 12263-12271.
7. “Biocompatible phosphate anchored Fe3O4 nanocarriers for drug delivery andhyperthermia P. Sharma, Suman Rana, K. C. Barick and P. A. Hassan*New J. Chem.* 2014, 38, 5500-5508.
8. “Folate-conjugated luminescent Fe3O4 nanoparticles for magnetic hyperthermia”K. C. Barick, Suman Rana and P. A. Hassan*AIP Conf. Proceedings* 2013, 1591, 561-562.iv
9. “Microstructural investigation of lipid solubilized microemulsions using laser light scattering”Suman Rana, G. Verma and P. A. Hassan*Adv. Mat. Lett.* 2013, 4, 476-481.

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122. Name : **Brindaban Modak**
Enrolment No. : CHEM01201004003
Date of Award of degree : 15.11.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Theoretical Studies on Materials for Hydrogen Energy Applications.

Abstract

The present thesis focusses on three important aspects related the hydrogen economy viz., designing efficient strategy for generation of hydrogen, developing cost effective, durable, safe, and environment friendly storage system, and designing infrastructure for application of hydrogen. Using the density functional theory (DFT) based electronic structure calculations, we have designed perovskite based photocatalysts for the generation of hydrogen via visible light driven water splitting. To develop efficient materials for hydrogen storage, we have investigated different light metal decorated porous carbon nanostructures which can absorb molecular hydrogen. Finally, calculations for designing new materials for the efficient oxygen reduction reaction have been carried out. All these discussions are presented in the eight chapters of the thesis.For the generation of hydrogen via visible light driven water splitting, detailed DFT based electronic structure calculations have been carried out by doping suitable dopant atoms into perovskite based photocatalyst materials. The various important dopant pairs such as (N,Mo), (N,F), and (Sb, N), (Rh, Sb) are used for $NaTaO_3$ and $SrTiO_3$ respectively. Another material studied for this purpose is metal decorated porous graphitic carbon nitride (g-C_3N_3). For the computational design of hydrogen storage materials, metal decorated porous graphitic carbon nitride (g-C_4N_3) has been predicted to be a possible hydrogen storage material with the feasibility of operation at ambient temperature and pressure. For designing new catalyst for oxygen reduction reaction, which is an important limiting step in fuel cell application, metal decorated porous carbon nitride fullerene has been considered.

Publications

Journal

1. Photocatalytic Activity of $NaTaO_3$ Doped with N, Mo, and (N,Mo): A Hybrid Density Functional Study. Brindaban Modak, K. Srinivasu and Swapan K. GhoshJ. Phys. Chem. C 2014, 118, 10711 − 10719.
2. Band Gap Engineering of $NaTaO_3$ by Density Functional Theory: A Charge Compensated Codoping Strategy. Brindaban Modak, K. Srinivasu and Swapan K. Ghosh Phys. Chem. Chem. Phys. 2014, 16, 17116−17124.
3. A Hybrid DFT Based Investigation of the Photocatalytic Activity of Cation–Anion Codoped $SrTiO_3$ for Water Splitting under Visible Light. Brindaban Modak, K. Srinivasu and Swapan K. GhoshPhys. Chem. Chem. Phys. 2014, 16, 24527-24535.
4. Improving Photocatalytic Properties of $SrTiO_3$ through (Sb, N) Codoping: A Hybrid Density Functional Study. Brindaban Modak, K. Srinivasu and Swapan K. GhoshRSC Adv. 2014, 4, 45703–45709.
5. Improvement of Photocatalytic Activity of $NaTaO_3$ under Visible Light by N and F Doping. Brindaban Modak, and Swapan K. GhoshChem. Phys. Lett. 2014, 613, 54–58.
6. Role of F in Improving the Photocatalytic Activity of Rh-Doped $SrTiO_3$. Brindaban Modak, and Swapan K. GhoshJ. Phys. Chem. C 2015, 119, 7215−7224.
7. Origin of Enhanced Visible Light Driven Water Splitting by (Rh, Sb)-$SrTiO_3$. Brindaban Modak, and Swapan K. GhoshPhys. Chem. Chem. Phys. 2015, 17, 15274-15283.
8. Exploring The Role of La Codoping beyond Charge Compensation for Enhanced Hydrogen Evolution by Rh-$SrTiO_3$. Brindaban Modak, and Swapan K. Ghosh J. Phys. Chem. B 2015, 119, 11089−11098.
9. Enhancement of Visible Light Photocatalytic Activity of $SrTiO_3$: A Hybrid Density Functional Study. Brindaban Modak, and Swapan K. GhoshJ. Phys. Chem. C 2015, 119, 23503−23514.
10. Improving Visible Light Photocatalytic Activity of $KNbO_3$ by using (N, W) as an Efficient Dopant Pair Brindaban Modak, and Swapan K. Ghosh RSC Adv. 2016, 6, 9958–9966.
11. An Efficient Strategy for Controlled Band Gap Engineering of $KTaO_3$ Brindaban Modak, and Swapan K. GhoshJ. Phys. Chem. C 2016, 120, 6920−6929.
12. Improving The Photocatalytic Activity of S-Triazine Based Graphitic Carbon Nitride through Metal Decoration: An ab Initio Investigation.K. Srinivasu, Brindaban Modak, and Swapan K. GhoshPhys. Chem. Chem. Phys. 2016,18, 26466-26474.

13. Improving Visible Light Photocatalytic Activity of $NaNbO_3$: A DFT based Investigation Brindaban Modak, Pampa Modak and Swapan K. Ghosh RSC Adv. 2016, 6, 90188–90196.
14. Improving Visible Light Photocatalytic Activity of $KTaO_3$ using Cation-Anion Dopant Pair.Brindaban Modak, and Swapan K. Ghosh Sol. Energy Mater Sol. Cells 2016, (Accepted).
15. Exploring Metal Decorated Porphyrin-like Porous Fullerene as Catalyst for Oxygen Reduction Reaction: A DFT StudyBrindaban Modak, K. Srinivasu, and Swapan K. GhoshInt. J. Hydrogen Energy (Under Review

Conferences

1. Improvement of Photocatalytic Activity of $NaTaO_3$ under Visible Light by Codoping with Mo, N: A Hybrid Density Functional Theory.Brindaban Modak, K. Srinivasu, and Swapan K. GhoshCurrent Trends in Theoretical Chemistry, BARC (CTTC-2013).
2. Hybrid Density Functional Study on (Sb, N) codoped $SrTiO_3$ with Improved Photocatalytic Property.Brindaban Modak, K. Srinivasu, and Swapan K. GhoshTrombay Symposium on Radiation & Photochemistry, (TSRP-2014), BARC
3. A Hybrid DFT Based Investigation of Tuning Band Gap: Compensated Vs Non-Compensated Codoping.Brindaban Modak, K. Srinivasu and Swapan K. GhoshProceedings of DAE-BRNS 5th Interdisciplinary Symposium on Materials Chemistry (ISMC-2014), BARC, [Best Poster Presentation Award (Second Prize)]
4. Improvement of Photocatalytic activity of $NaTaO_3$ by codoping with Nitrogen and Halogen.Brindaban Modak, and Swapan K. Ghosh. Proceedings of DAE-BRNS Symposium on Multiscale Modeling of Materials and Devices (MMMD-2014), BARC, Page-97.[Best Poster Presentation Award]
5. (Mo, N) Doping for Enhanced Photoelectrochemical Water Splitting of $SrTiO_3$.Brindaban Modak, K. Srinivasu and Swapan K. GhoshTheoretical Chemistry Symposium (TCS-2014), CSIR-NCL, Pune

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123. Name : **Sabyasachi Patra**
Enrolment No. : CHEM01201204007
Date of Award of degree : 15.11.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Investigation On Synthesis,Mechanism Of Formation And Catalytic Application Of Metal Nanoparticles In Nanoscale Confinement Of Polymer Matrices.

Abstract

The present thesis has been aimed at exploring some novel routes for the synthesis of noble metal nanoparticles in different polymer matrices, understanding their mechanism of formation and catalytic activity. Ion-exchange membranes and neutral polymeric resins have mostly been used as the host matrices for nanoparticle synthesis because of their nanoscale morphology. The synthesis of nanoparticles has been accomplished by two approaches: (i) the direct in-situ reduction of metal ions in the polymeric host and (ii) nanoconfinement driven reduction of metal ions in the polymeric host. State-of-the-art characterization techniques like small angle X-ray scattering (SAXS) and electron microscopy have been frequently used for the study of nanoparticle morphology as well as their time resolved formation and growth. 110mAg radiotracer has been employed as a marker for studying the time resolved evolution of silver nanoparticles in different membranes for the first time. Special emphasis has been given on understanding the role of nanoscale confinement of the host matrices on facilitating the chemistry of nanoparticle synthesis as well as the chemistry of nanoparticles mediated catalysis. Experiments have been carried out to investigate the possible origin of the so called “Nanoconfinement Effect” and havebeen explained in terms of reduced molecular mixing of the reactant and product states. The study sought to get answer of some of the fundamental questions like, (i) how to control the sizeand shape of metal nanoparticles stabilized in polymer matrices? (ii) how metal nanoparticles can be chemically impregnated into nanoporous polymer matrices at ambient condition irrespective of the chemical nature of the matrix, and (iii) how such nanoporous polymer-metal nanoparticles composites can acts as catalytic nanoreactor with enhanced activity.

Publications

Journal

1. Local conditions influencing in situ formation of different shaped silver nanostructures and subsequent reorganizations in ionomer membrane. S.Patra, D. Sen, A.K. Pandey, C. Agarwal, S.V. Ramagiri, J.R. Bellare, S.Mazumder, A. Goswami, *J. Phys. Chem. C* 2013, *17*, 12026–12037.
2. Synthesis, characterisation and counterion dependent mesoscopicmodifications of ionomer nanocomposites having different dimensional silvernanostructures. S. Patra, D. Sen, C. Agarwal, A.K. Pandey, S. Mazumder, A.Goswami, *AIP Conf. Proc.* 2013, *1512*, 230-231.
3. Time resolved growth of membrane stabilized silver NPs and their catalyticactivity. S. Patra, D. Sen, A.K. Pandey, J. Bahadur, S. Mazumder, S.V.Ramagiri, J.R. Bellare, S.V. Roth, G. Santoro, S. Yu, A. Goswami, *RSCAdvances* 2014, *4*, 59379–59386.
4. Redox decomposition of silver citrate complex in nanoscale confinement: an unusual mechanism of formation and growth of silver nanoparticles. S. Patra, A.K. Pandey, D. Sen, S.V. Ramagiri, J.R. Bellare, S. Mazumder, A. Goswami, *Langmuir* 2014, *30*, 2460−2469.
5. Silver Nanoparticles Stabilized in Porous Polymer Support: A Highly Active Catalytic Nanoreactor. S. Patra, A.N. Naik, A.K. Pandey, D. Sen, S.Mazumder, A. Goswami, *Applied Catalyis A: General* 2016, *524*, 214-222.

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124.	Name	:	**Nitin Minocha**
	Enrolment No.	:	ENGG01201104018
	Date of Award of degree	:	15.11.16
	Constituent Institute	:	Bhabha Atomic Research Centre,
	Title	:	Investigation On Synthesis,Mechanism Of Formation And Catalytic Application Of Metal Nanoparticles In Nanosc Confinement Of Polymer Matrices.

Publications

Journal

1. “Numerical investigation of three-dimensional natural circulation phenomenon in passive safety systems for decay heat removal in large pools.”, Minocha N., Joshi J. B., Nayak A. K.,Vijayan P. K.,*International Journal of Heat and Mass Transfer*, 2015, *81*, 659-680.
2. “3D CFD Simulation of passive decay heat removal system under boiling conditions: role ofbubble sliding motion on inclined heated tubes.”, Minocha N., Joshi J. B., Nayak A. K., Vijayan P.K., *Chemical Engineering Science*, 2016, *145*, 245-265.
3. “3D CFD simulation to study the effect of angle of inclination of condenser tube on naturalconvection and thermal stratification in a passive decay heat removal system.”, Minocha N., Joshi J.B., Nayak A. K., Vijayan P. K., *Nuclear Engineering and Design,* 2016, *305*, 582-603.

Conferences

1. “3D CFD Simulation of passive decay heat removal system under boiling conditions: role ofbubble sliding motion on inclined heated tubes.”, Minocha N., Joshi J. B., Nayak A. K., Vijayan P.K., *12th International Conference on Gas-Liquid and Gas-Liquid-Solid Reactor Engineering (GLS12)-2015.* June’ 28-July’ 1, 2015. Columbia University, New-York
2. “3D CFD simulation to study natural circulation phenomenon in Passive Safety Systems fordecay heat removal in large pools.”, Minocha N., Joshi J. B., Nayak A. K., Vijayan P. K., *Fluid Mechanics and Fluid Power-2014.* December’2014. Kanpur, India.
3. “Numerical investigation of multidimensional natural circulation phenomenon in Passive Safety Systems for decay heat removal in large pools.” Minocha N., Joshi J. B., Nayak A. K.Vijayan P. K., *New Horizons in Nuclear Thermal Hydraulics and Safety.* January’2014. Mumbai,India.
4. “Numerical investigation of multidimensional natural circulation phenomenon in PassiveSafety Systems for decay heat removal in large pools.” Minocha N., Joshi J. B., Nayak A. K.,Vijayan P. K., *New Horizons in Nuclear Thermal Hydraulics and Safety.* January’2014. Mumbai, India.

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125. Name : **Ekata Saha**
Enrolment No. : MATH10201204001
Date of Award of degree : 16.11.16
Constituent Institute : Institute of Mathematical Sciences,
0Title : Arithmetic Properties Of Generalised Euler-Briggs Constants.

Abstract

In his quest to assign a value for _(1), Euler introduced the constant as the limit

$$\gamma := \lim_{x\to\infty}\left(\sum_{1\le n\le x}\frac{1}{n} - \log x\right).$$

The above constant is now known as Euler's constant. Over the past _fty years, Euler's constanthas been generalised and studied by many mathematicians like Briggs, Lehmer, Murty, Saradha, Diamond and Ford. We now introduce the following generalisation of , which uni_es the families introduced by Briggs and Diamond-Ford. We refer to them as generalised Euler-Briggs constants.Let be a _nite subset of primes and a; q beas de_ned earlier. Then the generalised Euler-Briggs constant (; a; q) is de_ned by the followinglimit:

$$\gamma(\Omega, a, q) \ := \ \lim_{x\to\infty}\left(\sum_{\substack{n\le x\\ n\equiv a \bmod q\\ (n,P_\Omega)=1}} \frac{1}{n} \ - \ \delta_\Omega\frac{\log x}{q}\right).$$

This thesis is devoted to study various arithmetic properties of these constants, such as transcen-dence, linear independence over the _eld of rational numbers as well as over other number _elds and the _eld of algebraic numbers.

List of Publications arising from the thesis

(1) Transcendence of generalized Euler-Lehmer constants", Sanoli Gun, Ekata Saha and SnehBala Sinha, J. Number Theory, 2014, 145, 329-339.
(2) A note on generalized Briggs-Lehmer constants", Sanoli Gun and Ekata Saha, RamanujanMath. Soc. Lect. Notes Ser., 2016, 23, 93-104.
(3) Linear and algebraic independence of Generalized Euler-Briggs constants", Sanoli Gun,V.Kumar Murty and Ekata Saha, J. Number Theory, 2016, 166, 117-136.

Publications

Journal

1. “Transcendence of generalized Euler-Lehmer constants”, Sanoli Gun,Ekata Saha and Sneh Bala Sinha, J. Number Theory, 2014, 145, 329-339.
2. “A note on generalized Briggs-Lehmer constants”, Sanoli Gun andEkata Saha, Ramanujan Math. Soc. Lect. Notes Ser., 2016, 23, 93-104.
3. “Linear and algebraic independence of Generalized Euler-Briggs constants”,Sanoli Gun, V. Kumar Murty and Ekata Saha, J. Number Theory, 2016, 166, 117-136. Ekata

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126. Name : **Divyang G. Bhimani**
Enrolment No. : MATH08201004002
Date of Award of degree : 23.11.16
Constituent Institute : Harish-Chandra Research Institute
Title : Modulation Spaces And Nonlinear Evolution Equations.

Abstract

The study of the local and global well-posedness of non linear evolution PDE in spaces of low regularity represents one of the most active research fields, where the deepest machinery of modern harmonic analysis is applied. The principal aim of this PhD dissertation is to study nonlinear Schrödinger, wave and Klein-Gordon equations in the case of modulation $M^{p,q}(\ ^{d})$ and Wiener amalgam $W^{p,q}(\ ^{d})$ (time-frequency) spaces.In the last decade, many mathematicians have used these spaces as a regularity class for the Cauchy problem. In fact, fantastic progress have been done in the last decade from the PDE point of view in these spaces. But some of the fundamental issues were left open by active researchers in this field. For instance: (1) Whether one can take power type nonlinearity $u|u|^{\alpha}$ (α (0,∞) 2) in Schrödinger equation to obtain local well-posedness result? (2) The global well-posedness for the NLS with initial data (large) in modulation spaces has not yet clear due to lack of any useful conservation laws in these spaces by which one can guarantee global well-posedness.We obtain some sufficient conditions for nonlinearity uF(u) and |u| to be in $M^{1,1}$( ) whenever u $M^{1,1}$(and F is a contraction on .We study the Cauchy problem for Hartree type equations, that is, Schrödinger equations with cubic convolution nonlinearity $F(u)=K\ |u|^{2}$ under a specified condition on the potential K with Cauchy data on modulation spaces. We have established local and global well-posedness results for the Hartree type equations. In fact, these time-frequency spaces are present in various problems in the analysis, which also involves the study of twisted convolution. Finally, we take an excursion to the study of factorization problems with respect to twisted convolution in the realm of time-frequency and Lebesgue spaces. We have also illustrated its applications to functional analysis.

Publications

Journal

1. D.G. Bhimani, P.K. Ratnakumar, Functions operating on modulation spaces and nonlinear dispersive equations, J. Funct. Anal. 270 (2) (2016), 621-648. MR3425897.
2. D.G. Bhimani, The Cauchy problem for the Hartree type equation in modulation spaces, Nonlinear Anal. 130 (2016), 190-201. MR3424616.
3. D.G. Bhimani, Contraction of functions in modulation spaces, Integral Transforms Spec. Funct. 26, (9) (2015), 678-686. MR3354047.

Preprints

1. D.G. Bhimani, Composition operators on Wiener amalgam spaces. (Communicated)
2. D.G. Bhimani, On twisted convolution and modulation spaces. (In progress)

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127. Name : **Aparna Dilip Chaudhari**
Enrolment No. : LIFE09200904018
Date of Award of degree : 25.11.16
Constituent Institute : Tata Memorial Centre
Title : Role of galectin-3 in modulating tumor-specific immunity and lung metastasis in mice.

Abstract

Involvement of galectin-3 in various steps of cancer progression and metastasis has been extensively documented. However, how endogenous galectin-3 expression levels in the hostinfluence tumor growth and metastasis remains poorly understood till date. Further, the exact role of endogenous galectin-3 expression levels in the modulation of host anti-tumor immune responses and the mechanisms involved therein remain unclear and necessitatein-depthinvestigation.In the present thesis, role of endogenous galectin-3 in the regulation of host anti-tumor immunity and B16F10 lung metastasis was investigated using *LGALS3* transgenic mice,including Gal-3 wild type (Gal-3$^{+/+}$), Gal-3 hemizygous (Gal-3$^{+/-}$) and Gal-3 null (Gal-3$^{-/-}$) genotypic groups. Striking differences were observed in the immune scenario amongst these mice. Results indicated that, absenceof endogenous galectin-3 results in dysregulation of immune responses,reflected in increased T cell proliferation but reduced T cell Ca^{++} flux as well as ROS generationin stimulated splenocytes, decreased splenic NK cell frequency and NK cytotoxicity, markeddecrease in serum Thl,Th2 and Th17 cytokine levels with disturbed serum cytokines milieu, reduced serum IFN-γ concentration, low frequency of IFN-γRlexpressing splenic T and NK cells and attenuation of STAT1 mediated IFN-γ signaling in Gal-3$^{-/-}$ mice under normal physiological conditions. Experimental metastasis assay revealed that the ability of B16F10 murine melanoma cells to form lung metastatic colonies in Gal-3$^{+/+}$ and Gal-3$^{-/-}$ mice remained comparable and was significantly lower in Gal-3$^{+/-}$ mice.Under experimental metastasis assay conditions, Gal-3$^{-/-}$ mice splenocytes exhibited reduced NK cell frequency on day 14, higher proliferative responses, but reduced intracellular Ca^{++} flux and ROS generation upon *in vitro* stimulation. Further, the relative pattern of serum Th1, Th2 and Th17 cytokine concentrations in Gal-3$^{+/+}$, Gal-3$^{+/-}$ and Gal-3$^{-/-}$ mice changed gradually with the progression of lung metastasis.The enhanced B16F10 lung metastasis in Gal-3$^{-/-}$micecan be strongly attributed to the compromised anti-tumor immunityobserved in these mice.Overall the results suggested that, endogenous galectin-3 contributes to anti-tumor immune responses in the host. Endogenous galectin-3 expression levels in the host dictate the metastatic outcome through modulation ofhost immunity. Thefindingsprovided strong links to understand the crosstalk between galectin-3, immune system and cancer metastasis, which might facilitate the designing of more efficient galectin-3 targeted therapeutic strategies against cancer in the future.

Publications

Journal

1. 'Endogenous galectin-3 expression levels modulate immune responsesin galectin-3 transgenic mice', Aparna D. Chaudhari, Rajiv P. Gude, Rajiv D. Kalraiya andShubhadaV. Chiplunkar, *Molecular Immunology*,2015,68 (2):300-311.
2. 'Role of endogenous galectin-3 in regulation of anti-tumor immunityduring progression of B16F10 lung metastasis in galectin-3 transgenic mice', Aparna D. Chaudhariand Shubhada V. Chiplunkar. (Manuscript under preparation).

128. Name : **Swati Popat Phalke**
Enrolment No. : LIFE09200904011
Date of Award of degree : 25.11.16
Constituent Institute : Tata Memorial Centre
Title : Understanding the Crosstalk between Bone and Gamma Delta T lymphocytes In Cancer Patients

Abstract

Aminobisphosphonates are given as a standard treatment modality to patients with osteoporosis or with skeletal malignancies associated with breast cancer or multiple myeloma. The present thesis investigated the crosstalk and mechanism of action of aminobisphosphonate (Zoledronate) on breast tumor cells, immune cells (γδ T cells) and osteoclasts. The work embodied in the thesis demonstrated that activation status of the γδ T cells and cytokine dynamics (IFNγ/ IL6) dictates their anti or pro osteoclastogenic behavior. A proteomic approach using MALDI/TOF-TOF and LC-MS identified unique proteins and cellular pathways that were upregulated / downregulated in breast tumor cells after treatment with Zoledronate. Zoledronate created a ‘metabolic crisis’ in the breast tumor cells and induced apoptosis. The data obtained also identified molecules (IPP, HSPs and S100A8) that play an important role in γδ T cell mediated recognition of Zoledronate treated tumor cells. In the translational component of the thesis, immune profiles of the healthy individuals, treatment naïve breast cancer patients and Zoledronate treated breast cancer patients [who were exhibiting bone metastasis] were generated. Investigation of immune cell subsets, cytokine profiles, activation markers, memory markers and effector molecules on γδ T cells / αβ T cells was carried out using multicolor flow cytometry. The study demonstrated increased percentages of activated γδ T cells, majorly of terminally differentiated effector memory RA$^+$ type (TEMRA, highly cytotoxic), showing increased expression of CD25 and IFNγ in Zoledronate treated breast cancer patients. γδ T cells isolated from Zoledronate treated breast cancer patients also showed reduced IL6 secretion (pro-osteoclastogenic and pro-tumorigenic cytokine). The present study demonstrated that Zoledronate facilitates the tripartite crosstalk between the tumor cells, immune cells and bone cells and have also highlighted the effect of Zoledronate in breast cancer patients, which is significantly different from its well defined anti-resorptive function.

Publications

Journal

1. “Activation status of γδ T cells dictates their effect on osteoclast generation and bone resorption”, Swati P. Phalke, Shubhada V. Chiplunkar, “Bone Reports” (2015), Vol 3 (95-103)
2. “Cytokine dynamics of γδ T cells: A double edged sword in osteoclastogenesis”, Swati Phalke and Shubhada V. Chiplunkar, “Journal of Cytokine Biology” (2016), Vol 1, issue 3 (In Press)

129. Name : **Asif Amin Dar**
Enrolment No. : LIFE09201004005
Date of Award of degree : 25.11.16
Constituent Institute : Tata Memorial Centre
Title : Immune dysfunction in oral cancer patients: role of tumor Microenvironment.

Abstract

Oral cancer is the third most common cancer in India due to the high prevalence of tobacco chewing, smoking and alcohol consumption. Immune dysfunction appears to be more frequent and profound in cancer patients because of the accumulation of immunosuppressive factors /cells in the tumour microenvironment. The focus of the study was to identify factors secreted by oral tumours that affect the key T signaling events and to address the crosstalk of immunosuppressive cells such as myeloid-derived suppressor cells and regulatory T cells in inhibiting the antitumour immunity in oral squamous cell carcinoma (OSCC) patients.This study has unravelled different regulators which have the competency to dampen the antitumour immune response in oral cancer patients. For the first time, a potentially important function of tumour-derived OAS2 as a paracrine negative regulator of T-cell functions was identified. The mechanism employed by TNF-α, an important negative regulator of T cell function was also addressed. Blocking TNFR2 enhanced the TNF-α induced T cell dysfunction suggesting that use of antagonist ligands aimed at a single receptor, TNFR2 holds the potential for selectively turning off immunosuppressive microenvironment. However, at the same time, it might lead to TNF-α induced TCR signaling defect in antigen encountered T cells via TNFR1. The Notch signaling was found to be one of the positive regulators of T cell signaling and inhibiting this signaling was observed to affect the proximal as well as distal signaling molecules. The study provided insight into mechanisms that integrate TCR and cytokine signals to determine the outcome of T cell response and identified a central role for notch signaling in this process. Our data highlight novel molecular targets for the manipulation of T-cell dependent immunity with important implications for cancer immunotherapy.Tumour microenvironment is characterized by chronic inflammation and accumulation ofimmune suppressive cells like Myeloid derived suppressor cells (MDSCs) and regulatory T cells (Tregs). These cells are responsible for suppression of T cell activation and dampening anti-tumour immunity. MDSCs were elevated in human OSCC patients and showed that they contribute to immune suppression and their levels correlated with cancer stage. STAT3 played an important role in MDSC activation and accumulation in OSCC patients. OSCC patients had elevated Tregs and correlated with IL-10 produced by MDSCs. However, MDSCs did not induce the Treg generation in*in vitro* conditions. MDSCs induced TH17 generation and IL17 producing cells were higher in OSCC patients. This suggests that MDSCs contribute in enhancing the inflammation as well as inducing T cell tolerance in oral cancer patients. Understanding the mechanism of action of immune suppressive cell populations in OSCC patients is important in designing effective immunotherapeutic modality.

Publications

Journal

1. “Involvement of Notch in activation and effector functions of gamma delta T cells” Dimpu Gogoi, Asif A Dar, Shubhada V Chiplunkar, *Journal of Immunology* 2014 Mar; 192(5):2054-62. doi: 10.4049/jimmunol.1300369
2. “Insights into the relationship between toll like receptors and gamma delta T cell responses”Asif A Dar, Rushikesh S Patil, Shubhada V Chiplunkar, *Frontiers in Immunology* 2014 Jul; 5:366. doi: 10.3389/fimmu.2014.00366
3. “The Jekyll and Hyde story of IL17 producing γδT (Tγδ17) cells” Rushikesh S Patil, Sajad A Bhat, Asif A Dar, Shubhada V Chiplunkar, *Frontiers in Immunology* 2015 Jan*;* 6:37. doi: 10.3389/fimmu.2015.00037
4. “Extracellular 2’5’ Oligoadenylate synthetase 2 mediates TCR CD3-ζ chain downregulation via caspase 3 activation in oral cancer” Asif A Dar, Trupti N Pradhan, Dakshayni P Kulkarni, Sagar Shah, Kanury V Rao, Devendra A Chaukar, Anil K D’Cruz, Shubhada V. Chiplunkar, *Immunology*2016 Feb;147(2):251-64. doi: 10.1111/imm.12560. Epub 2015 Dec 27.

Conferences

1. Presented a Poster titled “Contribution of myeloid derived suppressor cells to immune suppression in oral tumour microenvironment” at “13th FIMSA Advanced Immunology Course” organized by PGIMER, Chandigarh , India (March 2016)
2. Presented a Poster titled “Targeting Myeloid-derived suppressor cells (MDSCs) to rejuvenate the antitumour immunity in oral cancer” at International conference on “New Ideas in cancer challenging the dogmas”organized by Tata Memorial Centre, India (February 2016)
3. Oral presentation titled “Crosstalk of myeloid derived suppressor cells and Regulatory T cells in oral cancer”at “42nd Annual Convention of Indian Immunology Society (IIS), **“**Immunology in 21st century and beyond**”,** Patna (October 2015)
4. Oral presentation/poster titled “Myeloid derived suppressor cells are key players of immune suppression in oral cancer patients”at “34th Annual Convention of Indian Association for Cancer Research (IACR), **“**Cancer Research: from Bench to the Bedside”, Jaipur (February 2015)
5. Presented a Poster titled “Mechanism of immune dysfunction mediated by HLA-DR $^{–/low}$ CD33 $^{+}$ CD11b $^{+}$ myeloid cells in oral cancer patients” at International conference on “Molecular pathways to therapeutics: Paradigms and challenges in Oncology” organized by Carcinogenesis foundation, USA (February 2015).
6. Presented a Poster titled “Immune dysfunction in patients with oral cancer: role of myeloid derived suppressor cells and regulatory T cells” at “Keystone Symposia “Inflammation, Infection and Cancer”, held at Fairmont Chateau, Whistler, Canada (March 2014)
7. Presented a Poster titled “Immunosuppressive role of myeloid derived suppressor cells and regulatory T cells in patients with oral cancer” at ‘IX-DAE BRNS Life Sciences Symposium LSS-2013’ on “Current Advances in Immunobiology and Cancer”, held at BARC, Mumbai (November 2013)
8. Presented a poster titled “Immune dysfunction in oral cancer patients: Role of tumour microenvironment” at “32nd Annual Convention of Indian Association for Cancer Research (IACR) and “International symposium: Infection and Cancer”, held at ACBR, New Delhi (February 2013)

130. Name : **Kartikey Kumar Yadav**
Enrolment No. : CHEM01201104023
Date of Award of degree : 30.11.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Studies on the separation of rare earths using solid phase extraction and liquid membrane techniques.

Abstract

in permanent magnets, lamp phosphors, catalysts, rechargeable batteries etc. Evaluation of the current scenario in the field of rare earths separation and purification including environmental concerns indicate towards an urgent need to develop effective and efficient processes which not only maximizes the separation but also minimizes the environmental hazard associated with the conventional processes. This thesis deals with the consolidated efforts to develop a novel extraction material and membrane based techniques for the separation of rare earths elements from aqueous media with improved efficiency and lesser organic waste release in aqueous streams compared to conventional techniques like solvent extraction and ion exchange.This thesis reports development of novel polyethersulfone based composite beadsencapsulating organic extractant (di-2-ethyl hexyl phosphoric acid (D2EHPA) and 2-ethyl hexyl phosphonic acid (EHEHPA)) to separate and purify rare earths (Yttrium, Dysprosium) from lean and secondary sources. The polymeric beads were synthesized by non-solvent phase inversion technique. The developed D2EHPA/EHEHPA encapsulated polymeric beads act as a better alternative to the ion exchange process in terms of kinetics and mass transfer with >97% Y(III) and Dy(III) recovery. The developmental work also involved evaluation of various additive to alter the beads internal morphology which can maximize the encapsulation and minimize the loss of extractant. Polyvinyl alcohol and multiwall carbon nanotube doped PES/D2EHPA beads have shown higher loading capacity (100mg of Dy/gram beads) in comparison to conventional solvent extraction process. These polymeric beads also have excellent stability and reusability under harsh experimental conditions (vigorous mixing, strong acidity >50% HCl/H2SO4 and 100 cycle application) with minimal loss of encapsulated extractant (<2%). Based on the batch experimental results, the developed polymeric beads were successfully deployed for the recovery of rare earths(100 g Yttrium) in continuous column operation mode, to establish its potential to industrial level scale up. Another important objective of the present work was to develop separation scheme for rare earths separation from aqueous solution utilizing hollow fibre membrane module. The workcarried out in this thesis has led to the development of a process for rare earths recovery (Dy from La and Sm) by employing hollow fibre membrane (HFM) contactor module having organophosphorus type of extractant. The results obtained indicate successful optimization of conditions for dysprosium purification by using HFM module from the mixed rare earths feed upto 98% purity and >85% recovery. Rare earths separation from aqueous phase was obtained by employing HFM module in two different mode of operation i.e. non-dispersive solvent extraction and hollow fibre supported membrane. The stability and reusability of the HFSLM was found tobe good even after 5 successive runs.

Publications

Journal

1. Studies on separation of rare earths from aqueous media by polysulfone beads containingD2EHPA as extractant, Kartikey K. Yadav, D.K. Singh, M. Anitha, L. Varshney and H.Singh, Separation and Purification Technology, 118 (2013) 350-358.

2. Solvent impregnated carbon nanotube embedded polymeric composite beads: Anenvironment benign approach for the separation of rare earths, Kartikey K. Yadav, K.Dasgupta, D.K. Singh, M. Anitha, L. Varshney and H. Singh, Separation and Purification Technology, 143 (2015) 115-124.

3. Dysprosium sorption by polymeric composite bead: Robust parametric optimization usingTaguchi method, Kartikey K. Yadav, K. Dasgupta, D. K. Singh, L. Varshney, H. Singh,Journal of Chrmatography A, 1384 (2015) 37-43.
4. Sorption behavior of Y(III) from chloride medium with polymer composites containing di-2-ethyl hexyl phosphoric acid and multiwall carbon nanotube, Kartikey K. Yadav, K.Dasgupta, D.K. Singh, M. Anitha, R.K. Lenka, L. Varshney, H. Singh, Separation Scienceand Technology, 50 (2015) 463-470.b. Accepted: Nonec. Communicated: 2d. Other Publications: 16.

BARC News Letter:

1. Thermal analysis of polyethersulfone based composite beads encapsulated with di-2-ethyl hexyl phosphoric acid, Kartikey K. Yadav, D.K. Singh S. Francis and L. Varshney, H.Singh, BARC Newsletter, Founder's Day Special Issue (2013), p. 358.
2. Studies on CNT doped D2EHPA impregnated polymeric beads for yttrium extraction, Kartikey K. Yadav, K. Dasgupta, D.K. Singh, M. Anitha, L. Varshney and H. Singh, BARC Newsletter, Founder's Day Special Issue (2013), p. 361.

International Conferences:

1. Recovery of uranium from phosphoric acid medium by polymeric composite beads encapsulating organophosphorus extractants, D.K. Singh, Kartikey K. Yadav, Lalit Varshney and H. Singh, GLOBAL-2013: International Nuclear Fuel Cycle Conference,September 29 – October 3, 2013, Salt Lake City, Utah, USA

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131. Name : **Shyam Kailashrao More**
Enrolment No. : LIFE09201004004
Date of Award of degree : 30.11.16
Constituent Institute : Tata Memorial Centre
Title : "Altered cell surface glycosylation and organ specific metastasis''

Abstract

Dissemination of cells from primary tumor to secondary non-contagious site is called metastasis. Despite of high death rate in cancer patients is due to metastasis still it is poorly understood because of its complexity and multistep nature. Cell surface molecules play a crucial role in all the steps of metastatic cascade. Tumor cells show several cell surface modifications associated with the metastatic phenotype, including changes in the cell surface glycosylation.Previous work in the lab has shown that polyLacNAc substituted β1, 6 branched N-oligosaccharides expressed on B16F10 promote lung specific metastasis via galectin-3 which is expressed in highest amounts on the lungs. In the present study, importance of this interaction was proved by using modified citrus pectin which compete with lactose and dominant negative inhibitor truncated galectin-3 which compete with endogenous galectin-3.To prove that polyLacNAc on tumor cells indeed brings about these effects via galectin-3; galectin-3 transgenic mice were used. The decreased metastasis of B16F10 cells correlates with galectin-3 expression on the lungs in galectin-3$^{+/+}$ and galectin-3$^{+/-}$mice. However, galectin-3$^{-/-}$ mice showed comparable number of colonies to galectin-3$^{+/+}$ mice. While, surprisingly reversal of metastasis in gal-3$^{-/-}$ mice suggest host anti-tumor immunity may be compromised in these mice.In order to investigate the role of galectin-3, in our lab mass spectrometric screen was performed to find out galectin-3 binding proteins. It was found that along with many other cell surface glycoproteins, CD147 is a major carrier of β1,6 branched N-oligosaccharides. It is found to be localized in the cytoplasm after mutating all glycosylation sites. The critical glycosylation sites required for membrane targeting of CD147 were identified.Galectin-3 is a nucleo-cytoplasmic protein which is secreted out in a non-classical manner and often gets incorporated into the extracellular matrix component and basement membrane. The present study demonstrates thatdynamics and organization of lamellipodial structures formed and signaling events for their formation on galectin-3 are very distinct as compared to those observed on very well studied extracellular matrix component such as fibronectin.

Publications

Journal

1. S.K. More, S.V. Chiplunkar, R.D. Kalraiya, *Galectin-3 induced cell spreading and motility relies on distinct signaling mechanisms compared to fibronectin,*Molecular and Cellular Biochemistry, 416(2016)179-91.
2. S.K. More*, N. Srinivasan*, S. Budnar, S.M. Bane, A. Upadhya, R.A. Thorat, A.D. Ingle, S.V. Chiplunkar, R.D. Kalraiya, *N-glycans and metastasis in galectin-3 transgenic mice*, Biochemical and biophysical research communications, 460 (2015) 302-307 (*Equal Contribution).
3. A.K. Agarwal, N. Srinivasan, R. Godbole, S.K. More, S. Budnar, R.P. Gude, R.D. Kalraiya, *Role of tumor cell surface lysosome-associated membrane protein 1 (LAMP1) and its associated carbohydrates in lung metastasis*, Journal of cancer research and clinical oncology, 141(9) (2015) 1563-74.
4. M.C. Dange*, N. Srinivasan*, S.K. More, S.M. Bane, A. Upadhya, A.D. Ingle, R.P. Gude, R. Mukhopadhyaya, R.D. Kalraiya, *Galectin-3 expressed on different lung compartments promotes organ specific metastasis by facilitating arrest, extravasation and organ colonization via high affinity ligands on melanoma cells*, Clinical & experimental metastasis, 31 (2014) 661-673 (*Equal Contribution).

Presentation at conferences

1. Presented poster titled Galectin-3 mediated cell spreading and movement utilizes distinct molecular mechanisms compared to those used on fibronectin in "*Molecular Pathways to Therapeutics: Paradigms and Challenges in Oncology*", Carcinogenesis 2015, International conference organized by Carcinogenesis Foundation, USA and TMC-ACTREC, India on Feb-2015, TMC-ACTREC, NaviMumbai.
2. Presented poster titled Identification of galectin-3 binding proteins carrying poly-*N*-acetyllactosamine (polyLacNAc) substituted β1, 6 branched N-oligosaccharides on melanoma cells to elucidate their role in lung specific metastasis in National Conference on "*Glycobiology of Cancer; Lectins as tools and Targets*", Nov 2013, KarnatakUniversity.
3. Presented poster titled Galectin-3 on the lungs and melanoma metastasis in National Conference on "*Glycobiology of Cancer; Lectins as tools and Targets*", Nov 2013, KarnatakUniversity.

132. Name : **Aditi Kamlesh Sahu**
Enrolment No. : LIFE09201004007
Date of Award of degree : 30.11.16
Constituent Institute : Tata Memorial Centre
Title : Raman Micro-Spectroscopy Studies of Oral Cancerous and Premalignant Conditions.

Abstract

Oral cancer is the sixteenth most common cancer in the world and the most common malignancy in Indian men. The survival rates for oral cancer have not improved in several decades. Delays in diagnosis and recurrences are the major causes for the low survival rates. Visual inspection followed by biopsy and histopathological examination is the gold standard for oral cancer diagnosis; however these approaches have associated limitations. As early diagnosis can improve survival rates and overall patient outcomes, there is a need to develop rapid, objective and patient friendly less-invasive/ non- invasive approaches for screening and early diagnosis. Raman spectroscopy (RS), a vibrational spectroscopic approach based on inelastic scattering of light, has shown promise in cancer diagnosis. In the present study, the potential of RS in early oral cancer diagnosis and sub-site classification was explored using both ex vivo (serum and exfoliated cells) and in vivo approaches. Serum RS was explored for oral cancer diagnosis and sub-site classification using both resonance (n=70) and conventional Raman (n=86) studies. Similar classification was observed for normal and oral cancer groups, even buccal mucosa and tongue cancers could be classified. Further, potential of serum RS in screening was observed using 339 samples where normal could be distinguished from other disease conditions (premalignant, disease control and oral cancer) with sensitivity and specificity values comparable to existing screening approaches like Pap and mammography. Exfoliated cells collected from healthy without tobacco (n=40), healthy with tobacco (n=40), oral premalignant (n=27) and malignant subjects (n=31) were subjected to Raman spectra acquisition and Pap staining (for cytological correlation). These samples were analyzed in two different studies; *proof-of-concept* where differences between healthy and oral cancer were explored and *early diagnosis* where feasibility to detect premalignant cells was evaluated. Healthy could be successfully differentiated from tumor cells; lower classification was observed in premalignant samples. In vivo studies were undertaken as a non-invasive modality to diagnose cancer at different subsites: buccal mucosa, lip and tongue using healthy (n=72) and oral cancer subjects (n=85). In the first step, anatomical differences between these three subsites were evaluated in healthy, contralateral, premalignant and malignant conditions. Subsequently, diagnostic algorithms to distinguish healthy, contralateral, premalignant and malignant conditions were built for individual and then pooled subsites. The pooled subsites approach was found to be more meaningful for screening applications. Thus, studies in this thesis have demonstrated potential of RS in oral cancer diagnosis and screening using both less-invasive and non-invasive approaches. Large-scale clinical and field trials are important before prospective clinical translation can be realized.

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1. In vivo sub-site classification and diagnosis of oral cancers using Raman spectroscopy, Aditi Sahu, Arti R. Hole, Atul Deshmukh, Sudhir Nair, Pankaj Chaturvedi, C. Murali Krishna, JIOHS, 9 (5), 2016
2. Oral cancer screening: A serum Raman spectroscopic approach, Aditi Sahu , Suyash Dhoot, Amandeep Singh, Sharada S. Sawant, Nikhila Nandakumar, Sneha Talathi-Desai, Mandavi

Garud, Sandeep Pagare, Sanjeeva Shrivastava, Sudhir Nair, Pankaj Chaturvedi, C. Murali Krishna, JBO, 20 (11), 2015

3. Raman spectroscopy and cytopathology of oral exfoliated cells for oral cancer diagnosis, Aditi Sahu, Sneha Tawde, Venkatesh Pai, Poonam Gera, Pankaj Chaturvedi, Sudhir Nair, C. Murali Krishna, Ana Met, 7, 2015.
4. "Raman spectroscopy of serum: a study on oral cancers", Aditi Sahu, Sneha Talathi, Sharada Sawant and C. Murali Krishna, Biomed Spectro Imaging, 4(2), 2015.
5. "Recurrence prediction in oral cancers: a serum Raman spectroscopy study", Aditi Sahu, Nikhila Nandakumar, Sharada Sawant and C. Murali Krishna, Analyst 140(7):2294-301, 2015.
6. "Raman spectroscopy and oral exfoliative cytology", Aditi Sahu, Nupur Shah, Manoj Mahimkar, Mandavi Garud, Sandeep Pagare, Sudhir Nair, C. Murali Krishna, Proc SPIE 89262N-89262N-4, 2014.
7. "Classification of oral cancers using Raman spectroscopy of serum", Aditi Sahu, Sneha Talathi, Sharada Sawant, C. Murali Krishna, Proc SPIE 89390E-89390E-7, 2014.
8. "Raman spectroscopy of serum: an exploratory study for detection of oral cancers", Aditi Sahu, Sharada Sawant, Hitesh Mamgain, C. Murali Krishna., Analyst, 2013.
9. "In vivo Raman spectroscopy of oral buccal mucosa: a study on malignancy associated changes (MAC)/cancer field effects (CFE)", S.P.Singh, Aditi Sahu, Atul Deshmukh, Pankaj Chaturvedi, C. Murali Krishna., Analyst, 2013.
10. "Raman spectroscopy of oral buccal mucosa: a study on age-related physiological changes and tobacco-related pathological changes", Aditi Sahu, Atul Deshmukh, A.D. Ghanate, S.P. Singh, Pankaj Chaturvedi, C. Murali Krishna, Technol Cancer Res Treat. 11, 529-541 (2012).

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1. Presented a poster entitled "A Raman spectroscopy approach for classification of subsites in oral cancers: A feasibility study", *Aditi Sahu,* S.P. Singh, Atul Deshmukh, Pankaj Chaturvedi, C. Murali Krishna (also selected as a proferred talk) at AACR 2011, New Delhi
2. Presented a poster entitled" "Serum based diagnosis of asthma: a Raman spectroscopic approach", *Aditi Sahu,* Krishna Dalal, Sarla Naglot, and C. Murali Krishna, at ICORS 2012, Bangalore
3. Presented a poster entitled "To explore utility of Raman spectroscopy in therapeutic drug monitoring of Imatinib", Vikram Gota, *Aditi Sahu,* Anand Patil, and C. Murali Krishna at ICORS 2012, Bangalore
4. Poster presentation entitled, "Raman spectroscopy and oral exfoliative cytology: Investigating misclassifications between contralateral normal and tumor sites", *Aditi Sahu,* S. Tawde, Poonam Gera, S. Nair, C. Murali Krishna in TMC Platinum Jubilee Conference, Mumbai, 2016
5. Poster presentation entitled, "Serum Raman spectroscopic classification of buccal mucosa and tongue cancers", *Aditi Sahu,* Sneha Talathi-Desai, Sharada Sawant, C. Murali Krishna at OWLS, TIFR, Mumbai, 2016.

133. Name : **Komal Chandra Shrivastava**
Enrolment No. : CHEM01201004012
Date of Award of degree : 1.12.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Physico-Chemical Investigations Of Different Materials Of Relevance In Nuclear Technology.

Abstract

The work carried out in present thesis mainly focused on diffusion behaviour of hydrogen and deuterium in Zr based alloys to understand deuterium ingress in pressure tubes of Pressurised Heavy Water Reactors (PHWRs), development of analytical methodology for determination of total gas in Prototype Fast Breeder Reactor (PFBR) fuel material, studies on the possible use of Pd nanocatalyst for reduction of U(VI) to U(IV) in fuel reprocessing.The work carried out has been elaborated in four topics of the thesis.Topic one gives a brief overview of pick-up of hydrogen and deuterium in Zircaloy based materials used as a coolant channel in PHWRs**.** The determination of hydrogen and deuterium in Zr-2.5%Nb Pressure tube material was done simultaneously by HVE-MS. Actual irradiated Zr-2.5%Nb coolant channel samples were analyzed for their hydrogen and deuterium content. Topic two describes the determination of diffusion coefficient of hydrogen and deuterium in Zr-2.5%Nb material used for manufacturing the pressure tubes in PHWRs. Diffusion Coefficient of Hydrogen was found to be higher than Deuterium. However, the activation energies for hydrogen and deuterium were found to be nearly the same (~35 kJ/mol). The frequency factor for hydrogen was higher than for deuterium by a factor of 2.3, which is in line with the mass dependence (1/ m) of jump frequency. Topic three deals with the formation of Pd nanoparticles anchored on Fe_3O_4 and SiO_2 particles using a new synthetic route and characterization of thus formed Pd NPs. Experimental studies on **t**he catalytic activities of the Pd NPs on the host SiO_2 and Fe_3O_4 particles in the reductions of Cr(VI) ($Cr_2O_7^{2-}$) and U(VI) (UO_2^{2+}) ions with formic acid were carried out. Hydrogen sorption properties of Pd NP's embedded on Fe_3O_4 and SiO_2 particles were determined with the help of Sievert's Apparatus. Topic four describes the determination of total gas content and it's composition in PFBR blanket pellets. A number of parameters such as temperature, duration of heating for quantitative extraction of evolved gases, total volume of the system, gas analysis condition etc. were optimized for reliable measurements. In addition, Sensitivity factors of H_2, CH_4, N_2, CO, O_2 and CO_2 in quadrupole mass spectrometer were determined for the quantification of the analytical results.

Publications

Journal

1. "Determination of Deuterium Pick-Up in Zr-Nb Alloy by Hot Vacuum Extraction-Quadrupole Mass Spectrometry", Komal Chandra, P. S. Ramanjaneyulu, C. S. Yadav, A. S. Kulkarni, Y. S. Sayi, K. L. Ramakumar, Analytical Letters, 2012, 45, 2136–2147.
2. "Determination of total gas content and its composition in Indian PFBR blanket pellets", P. S. Ramanjaneyulu, Komal Chandra, A. S. Kulkarni, C. S. Yadav, Abhijit Saha, M. K. Saxena, B. S. Tomar, K. L. Ramakumar, J Radioanal. Nucl. Chem., 2014, 301, 117–124.
3. "Determination of diffusion coefficients of hydrogen and deuterium in Zr-2.5%Nb pressure tube material using hot vacuum extraction – quadrupole mass spectrometry", Komal Chandra Shrivastava, A. S. Kulkarni, P. S. Ramanjaneyulu, Saurav Sunil, M. K. Saxena, R. N. Singh, B. S. Tomar, K. L. Ramakumar, J. Nucl. Mater., 2015, 461, 151–156.

4. "Palladium Nanoparticles Hosted on Hydrazine-grafted Magnetite and Silica Particles for Catalyzing the Reduction of Oxymetal Ions with Formic Acid", Komal Chandra Shrivastava, Sankararao Chappa, Arijit Sengupta, Amit P. Srivastava, Ashok K. Pandey, K. L. Ramakumar, Chem. Cat. Chem., 2016, 8, 2981-2987.

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1. "Determination of Deuterium content in irradiated Zirconium alloy - Ageing Management", C. S. Yadav, P. S. Ramanjaneyulu, Komal Chandra, A. S. Kulkarni, Y. S. Sayi, K. L. Ramakumar, RAPT – 2010, Anupuram, Chennai.
2. "Determination of Deuterium by HVE-QMS for Life Time Assessment of Zr-2.5%Nb Coolant Channels", K. L. Pandey, A. S. Kulkarni, Komal Chandra, P. S. Ramanjaneyulu, C. S. Yadav, Y. S. Sayi, K. L. Ramakumar, NUCAR 2011, Visakhapatnam, INDIA.
3. "Determination of total gas content and its composition in PFBR Blanket Pellets", P. S. Ramanjaneyulu, Komal Chandra, A. S. Kulkarni, C. S. Yadav, M. K. Saxena, K. L. Ramakumar, NUCAR 2013, Jabalpur, INDIA.
4. "Determination of Activation Energy of Hydrogen Diffusion in Zr-2.5%Nb Alloy", Komal Chandra, A. S. Kulkarni, P. S. Ramanjaneyulu, Sourav Sunil, C. S. Yadav, M. K. Saxena, R. N. Singh, B. S. Tomar, K. L. Ramakumar, THERMANS 2014 , TSH, BARC, Mumbai, INDIA.
5. "Thermal Conditioning of Palladium Nanoparticles Loaded Fe_3O_4", Komal C. Shrivastava, M. Phanindrakumar, S. K. Sali, K. L. Ramakumar, THERMANS 2016, DEPARTMENT OF PHYSICS,INDIAN INSTITUTE OF TECHNOLOGY, B.H.U., Varanasi, INDIA.

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134. Name : **Hirakendu Basu**
Enrolment No. : CHEM01201204013
Date of Award of degree : 5.12.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Synthesis And Characterization Of Hybrid Materials And Their Application For Decontamination Of Groundwater From Heavy Metals And Radionuclides..

Abstract

The contamination of groundwater by heavy metals originating either from natural soilsources or from anthropogenic sources is a matter of utmost concern to the public health.Remediation of contaminated groundwater is of highest priority since billions of people all over the world use it for drinking purpose. Depending on local geology, groundwater contains heavy metals (including radioactive elements) in low levels, but sometimes in concentrations which are not acceptable for drinking water. These heavy metals may be radioactive or even nanoparticles. They are not biodegradable and tend to accumulate in living organisms, causing various diseases and disorders. Treatment processes for contaminated ground water include filtration, centrifugation, chemical precipitation,coprecipitation, micro- and ultra filtration, sedimentation and gravity separation, flotation, coagulation, oxidation, solvent extraction, evaporation, distillation, reverse osmosis, ion exchange, electrolysis, adsorption etc. Adsorption is considered as one of the suitable water treatment methods due to the availability of a wide range of adsorbents and its ease of operation. Adsorption can be applied for the removal of organic, inorganic, and biological pollutants both in soluble and insoluble forms. Generally, packed bed columns, with a stable, porous material that has a specific grain size, are used. In spite of these facts, adsorption has certain limitations such as it could not achieve a good status at commercial levels. Probably, it is due to the lack of suitable adsorbents of high capacity to prepare commercial scale columns and a single adsorbent cannot be used for all kind of contaminants. Moreover, tailored materials must be stable and resistant to the medium that is investigated

so that there is no release of constituent components. Therefore cost effective alternative technologies or sorbents for treatment of contaminated groundwater are need of the modern days. The high 2 sorption capability exhibited by many biogenic material such as algae, bacteria, and yeasts or geological materials like silicate and aluminate could be exploited to develop a cost effective method for treating such waters. These geogenic and biogenic matrices can be tailored by chemical modification or by incorporation of suitable material in the matrix. This will not only make them specific to some metal ions or radionnuclides but will also enhance their sorption capacity. Composites consisting of two different components are called hybrid materials. Normally one component is inorganic in nature and the other is organic. Combining a inorganic matrix with biological systems offers important advantages. Algae appear to be one of the very promising materials in this regard. Dried algae or even algal extraction residues can be used as sorption material or for immobilizing the specific sorbent. The hybrid materials synthesis by impregnating inorganic material in organic matrices or vice versa shows enhances applicability in wastewater treatment. Hybrid materials could not only be effective in the removal of inorganic pollutants but also show fair affinity towards the radioactive and nanoparticle impurities as well. In general, these materials possess two different sorption sites enabling enhanced capability for removal. Another major advantage associated with these hybrid materials is that they will not leach into experimental solution as they do not have sufficient solubility in ground water in the pH range of 5-8. In view of this they can easily be separated from the process water. This can be verified by quantifyingvarious drinking water quality parameters after decontamination. This will ensure the safe consumption of drinking water by human beings. During this thesis work displacement reaction was used for immobilizing different materials in biogenic matrices. The porosity and the degree of immobilization of the embedded materials was controlled over a wide range of concentration. Core-shell types of hybrid materials were synthesized using sol-gel route. A 3 third category of hybrid material i.e. organic coating on inorganic substrate was also prepared. The resultant hybrid materials were characterized by using various techniques like Zeta-sizer for size characterization, SEM-EDS, FTIR, BET surface area analysis and XRD for the surface and structural characterization. The stability of the prepared hybrid material and changes in the properties were observed with time. The structure and binding capacity of different types of hybrid material was investigated with regard to their practical use for the selective and reversible accumulation of heavy metals and radionuclides. Detailed analysis of various metal ions was done by using absorption/emission spectroscopy while the ultra trace level of radionuclides was measured by using gamma and alpha spectrometry. This thesis aims at: (i) Development of highly efficient hybrid materials of different types (impregnation of suitable inorganic material into alginate matrix as well as core shell types), (ii) characterization of the newly developed hybrid material, (iii) removal of contaminants (conventional, radionuclides and nanoparticales) using the hybrid materials, (iv) practical field application of the developed hybrid materials. The hybrid materials developed and investigated in this thesis are: chitosan impregnated calcium alginate (for uranium); silica microspheres (for uranium, thorium); pure calcium alginate beads (for americium) and humic coated goethite (for americium and plutonium); silica microsphereimpregnated calcium alginate (for titanium oxide nanoparticle); goethite impregnatedcalcium alginate (for arsenic); alumina impregnated calcium alginate (for fluoride). The workdone and the obtained results are organised in following seven chapters.

Publications

Journal

1. Highly efficient removal of TiO2 nanoparticles from aquatic bodies by silica microsphereimpregnated Ca-alginate. H.Basu, R.K.Singhal, M.V.Pimple; New Journal of Chemistry,2016, 40, 3177—3186.
2. Arsenic removal from ground water by goethite impregnated calcium alginate beads.H.Basu, R.K.Singhal, M.V.Pimple, A.V.R.Reddy. Water, Air, and Soil pollution, 2015,226:22.
3. Synthesis and characterization of silica microsphere and their application in removal ofUranium and Thorium from water. H.Basu, R.K.Singhal, M.V.Pimple, A.V.R.Reddy.International Journal of Environmental Science and Technology, 2015, 12 (6), 1899-1906.

4. Development of natural sorbent for decontamination of drinking water from low level of transuranic and other long-lived radionuclides. R.K.Singhal, H .Basu , A.V.R.Reddy.Journal of Environmental Analytical Chemistry, 2014, 1:2.
5. Synthesis and characterization of alumina impregnated alginate beads for fluoride removalfrom potable water. H.Basu, R.K.Singhal, M.V.Pimple, A.V.R.Reddy. Water, Air, and Soil pollution, 2013, 224:1572
6. .Removal of environmental level of 239+240 Pu and 241Am from groundwater by using humiccoated colloidal suspension of goethite (α-FeO(OH)). R.K.Singhal, H.Basu,A.V.R.Reddy. Journal of Radioanalytical and Nuclear Chemistry, 2013, 295, 1345-1351.vi.
7. Removal of low level americium-241 from potable water originated from differentgeochemical environments by calcium alginate. R.K.Singhal, H.Basu, V.Manisha, A.V.R.Reddy, T. Mukherjee. Desalination 280, 2011, 313–318.

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1. Arsenic removal from ground water by goethite impregnated calcium alginate beads.H.Basu, R.K.Singhal, M.V.Pimple, and A.V.R.Reddy. Proceedings of the InternationalConference on Environmental Pollution and Remediation. Toronto, Ontario, Canada, July15-17, 2013.
2. Synthesis and characterization of silica microspheres and its use to remove traces of U, Th from potable water; H.Basu, R.K.Singhal, M.V.Pimple and A.V.R.ReddyProceedings ofNuclear and Radiochemistry Symposium. Govt. Model Science College, Jabalpur, India. Feb, 19-23, 2013

Communicated:

1. Chitosan impregnated Ca-alginate: A new hybrid material for removal of uranium frompotable water. **H. Basu**, R.K.Singhal, S.Saha, and M.V.Pimple.

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135. Name : **Benadict Rakesh**
Enrolment No. : CHEM02201004003
Date of Award of degree : 5.12.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Evaluation of tri-iso-amyl phosphate as an alternate extractant to tri-n-butyl phosphate for nuclear materials processing.

Abstract

Tri-*n*-butyl phosphate (TBP), a neutral organophosphorus extractant has been employed for several separation processes such as spent nuclear fuel reprocessing, monazite ore processing and Zr/Hf separation. However, TBP is susceptible to radiation and chemical degradation, more soluble in aqueous media than its higher homologues and forms third phase with tetravalent metal ions like Pu(IV), Th(IV) and Zr(IV). Earlier studies indicated that tri-*iso*-amyl phosphate (T*i*AP) is a potential alternate extractant to TBP for such processes. In this regard, the recent work has explored the feasibility of using T*i*AP based solvents for monazite ore processing and Zr/Hf separation.Determination of free acidity is crucial as it influences the extraction and third phase formation behaviour of a solvent and therefore, the reliable measurement of free acidity of U(VI) solutions using potassium oxalate - sodium fluoride as dual complexing agent is demonstrated over a wide range of U(VI):HNO_3 mole ratio. Also, methods for the determination of extractant concentration based on the measurement of density and refractive index of organic solutions have been reported. The extraction behaviour of T*i*AP and TBP based solvents with respect to metal ions such as U(VI), Th(IV), Nd(III), Zr(IV) and Hf(IV) are comparable. Third phase formation studies in the

extraction of Th(IV) and Zr(IV) in nitric acid media by T*i*AP and TBP based solvents showed a higher concentration of solutes and extractant in the third phase of TBP as compared to that of T*i*AP with increase in the diluent chain length, metal ion and HNO_3 concentrations. Small angle neutron scattering studies confirmed the higher aggregation tendency of TBP as compared to T*i*AP and also the attractive energy between the aggregates of TBP is higher as compared to that of T*i*AP.Extraction of metal ions from concentrated U(VI)-Th(IV)-Nd(III) feed solution in nitric acid media showed that the separation factor for Th(IV) with respect to other metal ions can be improved by employing T*i*AP based solvents. Furthermore, the T*i*AP based solvents resist organic phase splitting with concentrated Zr(IV)-Hf(IV) feed solution in nitric acid media. The overall results of extraction and third phase formation studies favour the deployment of T*i*AP based solvents in process plants for monazite ore processing and Zr/Hf separation.

Publications

Journal

1. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Studies on third phase formation in the extraction of $Th(NO_3)_4$ by tri-*iso*-amyl phosphate in *n*-alkane diluents. *Separation Science and Technology*, 2013, *48*, 2761-2770.
2. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Third phase formation in the extraction of $Th(NO_3)_4$ by tri-*n*-butyl phosphate and tri-*iso*-amyl phosphate in *n*-dodecane and *n*-tetradecane from nitric acid media. *Solvent Extraction and Ion Exchange,* 2014, *32*, 249-266.
3. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Extraction and stripping behaviour of tri-*iso*-amyl phosphate and tri-*n*-butyl phosphate in *n*-dodecane with U(VI) in nitric acid media. *Radiochimica Acta* 2014, *102* (7), 619-628.
4. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Compositional characterization of organic phases after the phase splitting in the extraction of $Th(NO_3)_4$ by 1.1 M tri-*n*-butyl phosphate/*n*-alkane. *Solvent Extraction and Ion Exchange,* 2014, *32*, 703-719.
5. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Separation of U(VI) and Th(IV) from Nd(III) by cross-current solvent extraction mode using tri-*iso*-amyl phosphate as the extractant. *Solvent Extraction and Ion Exchange,* 2015*, 33,* 448-461.
6. K. Benadict Rakesh, A. Suresh, N. Sivaraman, V.K. Aswal, P.R. Vasudeva Rao; Extraction and third phase formation behaviour of tri-*iso*-amyl phosphate and tri-*n*-butyl phosphate with Zr(IV) and Hf(IV) – A comparative study. *Journal of Radioanalytical and Nuclear Chemistry,* 2016*, 309* (3), 1037-1048.

National/International Conferences

1. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Third phase formation in the extraction of $Th(NO_3)_4$ by tri-*iso*-amyl phosphate (T*i*AP) in *n*-tetradecane. *Proceedings of biennial DAE – BRNS symposium on emerging trends in Separation Science and Technology (SESTEC-2012)*, Feb. 27 - March 1, 2012, Mithibai College, Vile Parle, Mumbai, Maharashtra, India, p 117.
2. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Extraction of U(VI) by 1.1 M tri-*iso*-amyl phosphate in *n*-dodecane from nitric acid media – Batch studies. *Proceedings of eleventh biennial DAE-BRNS symposium on Nuclear and Radiochemistry (NUCAR-2013)*, Feb. 19 – Feb. 23, 2013, Govt. Model Science College, R. D. University, Jabalpur, Madhya Pradesh, India, p 247.
3. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Comparison of third phase formation in the extraction of $Th(NO_3)_4$ by 1.1 M solutions of tri-*iso*-amyl phosphate and tri-*n*-butyl phosphate in *n*-dodecane from nitric acid media. *Proceedings of eleventh biennial DAE-BRNS symposium on Nuclear and Radiochemistry (NUCAR-2013)*, Feb. 19 - 23, 2013, Govt. Model Science College, R. D. University, Jabalpur, Madhya Pradesh, India, p 249.
4. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Compositional characterization of organic

phases after the phase splitting in the extraction of Th(IV) by 1.1 M tri-*n*-butyl phosphate/*n*-alkane. *Proceedings of biennial symposium on emerging trends in Separation Science and Technology (SESTEC-2014)*, Feb. 25 - 28, 2014, BARC Training School, Anushakthi Nagar, Mumbai, Maharashtra, India, p 95.

5. K. Benadict Rakesh, A. Suresh, N. Sivaraman, K. Nagarajan, P.R. Vasudeva Rao; Separation of U(VI) and Th(IV) from Nd(III) using tri-*iso*-amyl phosphate (T*i*AP) as the extractant – Batch Studies. *Fourth international conference on Asian Nuclear Prospects (ANUP-2014)*, Nov. 9-12, 2014, Lotte City Hotel, Jeju, Republic of Korea.
6. K. Benadict Rakesh, A. Suresh, P.R. Vasudeva Rao; Studies on third phase formation in the extraction of $Zr(NO_3)_4$ by solutions of tri-*iso*-amyl phosphate and tri-*n*-butyl phosphate in *n*-dodecane. *Chemistry in Nuclear Technology (CHEMNUT-2015),* July 30 - 31, 2015, Indira Gandhi Centre for Atomic Research, Kalpakkam, India.

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136. Name : **Issan Patri**
Enrolment No. : MATH10201004005
Date of Award of degree : 5.12.16
Constituent Institute : Institute of Mathematical Sciences,
Title : On some Group Theoretic, Ergodic Theoretic and Operator Algebraic Aspects of Compact Quantum Groups.

Abstract

In this thesis, we make study compact quantum groups from the viewpoint of group theory, ergodic theory and operator algebras. We define and study the notion of inner automorphisms of compact quantum groups and topological properties of the group of inner automorphisms of a compact quantum group. We show the stability of any normal subgroup of a compact quantum group under the action of an inner automorphism but show that the converse is false. We then define and study the center of compact quantum groups and compute it for several examples. This is followed by a study of group actions on compact quantum groups, where the action is by quantum group automorphisms. We investigate spectral properties of such non-commutative dynamical systems, which we call CQG dynamical systems, like ergodicity, weak mixing, etc and obtain combinatorial characterizations of such spectral properties, which enables us to construct examples which possess these properties. Under mild conditions, we also show the existence and uniqueness of a maximal ergodic normal subgroup of given CQG dynamical systems. Finally, we make a comprehensive study of the bicrossed product and the crossed product quantum groups, their representation theory and approximation properties possessed by such quantum groups like Haagerup property, weak amenability, etc. We discuss several examples and in particular, construct an infinite family of non-isomorphic quantum groups possessing Property (T).

Publications

Journal

1. Issan Patri, Normal subgroups, center and inner automorphisms of compact quantum groups, Internat.J. Math. 24 (2013), no. 9, 1350071, 37 pp.
2. Pierre Fima, Kunal Mukherjee and Issan Patri, On compact bicrossed products, To appear in JNCG,e-print available at arXiv:1504.00092.
3. Kunal Mukherjee and Issan Patri, Automorphisms of Compact Quantum Groups, submitted.

137. Name : **Rohan Raghava Poojary**
Enrolment No. : PHYS10200904001
Date of Award of degree : 5.12.16
Constituent Institute : Institute of Mathematical Sciences,
Title : Aspects of Holographic Induced Gravities.

Abstract

In recent years, AdS/CFT correspondance as emereged from string theory as one of the most powerful tools to study consistent theories of gravity by relating them to a boundary conformal field theory(CFT). It relates the partition function of the bulk (super)gravity in a locally Anti-deSitter(AdS) background to the generating function of corelators for the boundary CFT. With the boundary values of the fields in the bulk theory coupling as sources to the operators of the boundary CFT. Therefore the boundary conditions impossed on the bulk (super)gravity theory play an important role in determining the properties of the CFT.The most studied boundary condition were first introduced by Brown & Henneaux wherein they uncovered 2-copies of Virasoro algebra as the asymptotic symmetry algebra of AdS space in dim=3 (AdS_3) with central extension being *c=3//2G* with the boundary metric held fixed. These boundary conditions were later generalised to different settings of extended super-gravities and massless higher-spins fields (*hs)* in ADS_3. Here the super-Virasoro extensions and *W∞* were obtained as the asymptotic symmetry algebra respectively. The thesis concerns itself with consistently defining boundary conditions with fluctuating boundary values of the bulk fields and studiyng its implications in terms of the AdS_3/CFT_2 correspondance. AdS/CFT suggests that the boundary theory must be an Induced Gravity theory. Induced Gravity theories are generally obtained by coupling the CFT to the 2d background metric and integrating over the CFT degrees of freedom, thus obtaining a diffeomorphic invariant theory but which has Weyl anomalies. The thesis shows that the symmetries of such theories match with those of the bulk AdS_3 theories with boundary conditions which do not fix the boundary values of the bulk fields. This is done by first studying such boundary conditions in the pure gravity setting of AdS_3. These boundary conditions are susbsiquently generalised to extended super-gravities and massless *hs* fields. In each of these cases the asymptotic symmetry algebra of the Kac-Moody type are found for certain boundary conditions which are also the symmetries of certain Induced gravity theories.

Publications

Journal

1. S. G. Avery, R. R. Poojary and N. V. Suryanarayana "An sl(2,R) current algebra from AdS3 gravity" JHEP 1401 (2014) 144, arXiv: 1304.4252 [hep-th].
2. R. R. Poojary and N. V. Suryanarayana "Holographic chiral Induced W-gravities" JHEP 1510 (2015) 168, arXiv: 1412.2510 [hep-th].

138. Name : **Nirmalya Kajuri**
Enrolment No. : PHYS10200904004
Date of Award of degree : 5.12.16
Constituent Institute : Institute of Mathematical Sciences,
Title : Aspects of polymer quantization .

Abstract

Loop Quantum Gravity is an approach to Canonically quantize General Relativity. Where LQG succeeds over previous attempts in Canonical Quantization of the Gravitational field is in obtaining a kinematical Hilbert Space suitable for the theory. Briefly, this is done by taking SU(2) holonomiesas basic variables and using the Haar measure on SU(2) to define an inner product. This allows one to define an inner product invariant under spatial diffeomorphisms. A feature of LQG is that variables such as connection which are well defined classically, cannot be expressed as operators in the quantum theory. A related feature is that while finite diffeomorphisms arerepresented as unitary operators on the kinematical Hilbert space, their infinitesimal generators cannot be defined as operators.Analogous quantization techniques can be used for matter fields as well. In the context of quantizing point particles or scalar fields this is called polymer quantization. These theories share the above mentioned features of LQG that classical variables like position (for point particles) or the field (for scalar fields) do not exist as operators.The feature that generators of symmetries arenot defined as operators appears here as well. Out of this theories, the polymer quantized point particle (henceforth polymer quantum mechanics) can be regarded as either a toy model, or the correct theory of quantum mechanics - there is no justification from LQG in choosing one interpretation over the other. However, the polymer quantized scalar field theory has physicalrelevance from the LQG perspective. When one quantizes both matter fields and gravity, the usual Fock quantization which assumes a fixed background spacetime cannot be used and one must use a background independent quantization. For scalar fields, this is given by polymer quantization. According to LQG, the fundamental quantum description of a scalar field coupled toGravity is given by loop quantized gravitational field and polymer quantized scalar fields. In this thesis we have investigated certain aspects of polymer quantized theories. More specifically, we have investigated aspects in which the above mentioned features of absence of position (or field) variables as well as symmetry generators in the quantum theory play an important role. Wehave tried to answer the question of how these features make polymer quantized theories of scalar fields or point particles different from those obtained by the usual Schrodinger quantization.It is already remarkable and not well known that there exist discontinuous representations - representations of a Lie group which do not induce a representation of the corresponding Lie algebra. What is the physical relevance of this absence of symmetry generators? Is it an undesirable feature of the theory? This is one of the questions that our thesis investigates. Wesee that for the case of polymer quantized point particle, the discontinuity of the representations leads to infinite degeneracies. This is an undesirable feature and there are two escape routes. One is to break the symmetry, either explicitly or spontaneously. The other is to work in the dual space of the Hilbert space we started with - we find that the symmetry generators maybe defined in this space. This leads to an understanding of Polymer Quantization as an intermediate step in obtaining a physical theory. We carry out a similar investigation in case of polymer quantized scalar field theory and see that symmetry generators may be recovered in the dual space, just like the point particle case.As mentioned earlier, in LQG the fundamental description of a scalar field coupled to gravity is given by loop quantized gravitational field and polymer quantized scalar fields. However, in our semiclassical picture with fixed background spacetime, we employ Schrodinger quantization to describe scalar fields. It is important to ask how polymer and Schrodinger quantizations may be compared? In particular, if we consider a polymer quantized scalar field theory in a given background can it predict the same dynamics as a Schrodinger quantized scalar field? We have already noted that the field variable is unavailable as an operator for the polymer theory. One canhowever define an approximate field operator. What is the effect then of using approximate operators on the dynamics? In this thesis we address these questions by developing a path integral representation for polymer quantized scalar field theory. We

see that the path integral representation is very convenient to compare the two quantizations. We also see that the dynamics is indeed modified in the case of the polymer quantized theory due to the useof approximate field variables. In particular, we quantize a Klein Gordon field in Minkowski spacetime and nd that the resultant polymer quantized theory is not Lorentz invariant.

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139.	Name	:	**Santhosh**
	Enrolment No.	:	ENGG01200804015
	Date of Award of degree	:	13.12.16
	Constituent Institute	:	Bhabha Atomic Research Centre,
	Title	:	Development of Remaining Life Prediction Models for Instrumention and Control (I&C) Cables for use in Reliability Assessment of NPP Systems.

Abstract

Instrumentation and control (I&C) cables are one of the most important components in nuclear power plants (NPPs) because they provide power to safety-related equipment and also to transmit signals to and from various controllers to perform safety operations. The polymer materials used for insulation and jacket materials in I&C cables are susceptible to ageing and degradation mechanisms caused by exposure to many of the stressors encountered in NPP service conditions. Although, several condition monitoring and life estimation techniques are available, currently there is no standard methodology or an approach towards estimating the time dependent reliability of I&C cables. The state-of-the-art for incorporating the cable ageing effects into probabilistic safety assessment (PSA) is still evolving and current assumptions that need to be made on the failure rates and common cause effects are based on sparse data. Therefore, identification and quantification of ageing of electrical cables is very much essential for an accurate prediction of system reliability for use in PSA of NPPs. The objective of this thesis work is to develop a methodology to assess the susceptibility of polymeric cable insulation to various ageing mechanisms and to predict the state of the insulation at any chosen time in order to evaluate the remaining lifetime of operating cables in NPPs. In view of this, several concepts such as stress-strength interference (SSI) theory, artificial neural networks (ANNs) and Weibull theory have been employed to develop reliability prediction methodologies based on the measured performance indicators such as elongation at break (EAB), insulation resistance (IR) and oxidation induction time(OIT). A framework based on SSI theory has been developed to estimate the reliability of I&C cables from the measured IR by subjecting to thermal ageing. The methodology has been demonstrated for predicting the time dependent reliability of a typical I&C cable.

Another approach based on ANNs has been developed to predict the reliability of I&C cables from the initial readings of the IR measured during accelerated life testing. The methodology has been demonstrated with the accelerated life testing data on a typical I&C cable. In order to study the effect of thermal and radiation ageing in electrical cables, finite element analysis (FEA) simulations have been carried out. Study revealed that presence of aluminum screen in the cable can significantly contributes to the thermal degradation of insulation materials. FEA simulations have also been carried to study the impact voids, generated due to radiation ageing, on electrical parameters such as electric field, space charge density, etc. It was observed that the voids of size beyond 0.01mm radius have a significant effect on the electric field and other parameters. In order to assess the performance of cables received from various manufacturers and subsequent reliability prediction for use in PSA of NPPs, experimental studies such as IR measurement, EAB measurement, Fourier transform infrared (FTIR) spectroscopy, OITmeasurement, scanning electron microscopy (SEM) and positron annihilation lifetime spectroscopy (PALS) were carried out. The findings from differential scanning calorimetry (DSC) and FTIR are found to be in good agreement with the EAB findings. The SEM performed on fresh and aged samples also support the correlation from chemical and mechanical measurements. The PALS performed on fresh and irradiated samples also indicate generation of substantial free volume in the polymer matrix due to gamma radiation. From the performance indicators determined using experimental techniques, the time dependent reliabilities have been estimated by employing the proposed reliability approaches. Considering thesignificant increase in the unavailability of shutdown systemof Advanced Heavy Water Reactor (AHWR) with cable failure accounted, the overall study demonstrates that the cables connected to various NPP systems may be included in the PSA study.

Publications

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1. Remaining Life Prediction of I&C Cables for Reliability Assessment of NPP Systems, T. V. Santhosh, A. K. Ghosh and B. G. Fernandes, *Nuclear Engineering and Design*, 2012, no. 245, pp. 197– 201.
2. Reliability Prediction of I&C Cable Insulation Materials by DSC and Weibull Theory for Probabilistic Safety Assessment of NPPs, T. V. Santhosh, V. Gopika, A. K. Ghosh, B. G. Fernandes and K. A. Dubey, *Nuclear Engineering and Design*, 2015, no. 296, pp. 51-61.
3. Performance Assessment of I&C Cable Insulation Materials by DSC and SEM for NPP Ageing Management, T. V. Santhosh, A. K. Ghosh, B. G. Fernandes and K. A. Dubey, *International Journal of Systems Assurance Engineering and Management*, *Springer*, 2016, vol. 7, no. 1, pp. 6-15.
4. Lifetime Prediction of I&C Cables using OIT and OITp Measurements for PSA of NPPs, T. V. Santhosh, A. K. Ghosh and B. G. Fernandes, *Current Trends in Reliability, Availability, Maintainability and Safety: An Industry Perspective*, *Springer*, 2016, ISBN 978-3-319-23596-7.
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6. Condition Monitoring and Reliability Prediction of I&C Cables for use in Probabilistic Safety Assessment of NPPs, T. V. Santhosh, V. Gopika, A. K. Ghosh and B. G. Fernandes, *IEEE Transactions on Reliability*, 2016, Manuscript No. TR-2016-058, Revision submitted.
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140. Name : **Amit Kumar Das**
Enrolment No. : PHYS03200904002
Date of Award of degree : 13.12.16
Constituent Institute : Raja Ramanna Centre for Advanced Technology,
Title : Effects of disorder on electrical and optical properties of doped ZnO thin films grown by pulsed laser deposition.

Abstract

ZnO is a well known semiconductor which has been used for a long time in paints, sunscreen lotions, tooth paste, phosphor, varistor etc. However in recent past it has drawn the attention of semiconductor research community because it is a wide bandgap semiconductor with a bandgap of _ 3.38 eV at room temperature. By nature of its wide bandgap, ZnO is transparent in the entire visible spectral region. As a consequence, it is a suitable candidate for transparent conducting electrode applications and also as an active ingredient for novel and futuristic transparent electronic devices. Moreover being a direct bandgap semiconductor with its bandgap falling in the UV spectral region, it is also an efficient UV emitter. The large excitonic binding energy of _60 meV ensures that excitons can be present in ZnO even at room temperature that further enhances the UV emission efficiency. The excitonic nature of the near band edge emission makes ZnO a very good material for UV laser device applications. It can also be used in solar blind photo-detectors. Further ZnO has a very rugged wurtzite crystalline structure with a high cohesive energy which renders it radiation hard and high temperature stable. Therefore the ZnO based devices can be used in space and nuclear reactors and in applications that demand high temperature and high power handling. ZnO films and nanostructures have been grown by a variety of methods such as sol-gel, sputtering, MBE, MOCVD, electron beam evaporation, pulsed laser deposition (PLD), atomic layer deposition (ALD) etc. Among these PLD is a very simple and versatile technique that offers multiple advantages for growth of ZnO thin films and nanostructures. This technique uses high power pulsed laser at optimized fluence for ablating the target material to produce a luminous 11 plume that subsequently gets condensed on the suitable substrates placed in the path of the plume. No matter what growth method is used, the grown ZnO films will almost always have some degree of defects and disorders in it. These may be intrinsic point defects like zinc and oxygen interstitials and vacancies, unintentional impurities like H, Al, Ga etc. and structural disorders. Another important source of defects and disorder is the intentional doping of ZnO, required to tailor the electrical and optical properties. For example ZnO is doped with group III dopants such as Al, Ga, In, B, Si etc. to increase its electron concentration for applications in transparent conducting electrodes. Mg and Cd are introduced in ZnO for bandgap engineering. N, P, As, Sb, Li etc. are used as dopant for p-type conversion. The above mentioned defects and disorders in the doped/undoped ZnO films are randomly positioned throughout the film volume. The random potential fluctuations associated with disorder cause band tailing and bandgap narrowing. The free carriers released by the defects may bring about semiconductor to metal transition as well. The disorder in semiconductor lattice is also a source of carrier scattering that reduces their transport mean free path and mobility. If due to multiple scatterings from these randomly positioned defects the mean free path of the carriers becomes comparable to the Fermi wavelength, the carriers can no longer be considered as classical particles under effective mass approximations. In such cases quantum interference effects come into picture resulting in quantum corrections to the Boltzmann conductivity. Under these circumstances the low temperature transport properties of doped ZnO films get modified significantly. If the strength of disorder is very high, it may even cause strong localization of the carriers leading to metal to insulator transition and highly resistive ZnO films. Moreover the intentional or unintentional defects introduce trapping or luminescent levels in the ZnO bandgap resulting in defect related optical transitions which modify the photoluminescence and photoabsorption spectra. There exist numerous reports on the growth and characteristics of undoped and doped ZnO films. However systematic studies on the effects of disorder on the electrical and optical properties of doped ZnO thin films are needed for its practical applications. In the present thesis we have grown doped ZnO thin films 12 using optimized pulsed laser deposition. Their structural, electrical and optical properties have been characterized by high resolution X-ray di_raction (HRXRD), atomic force microscopy (AFM), photoluminescence (PL) and photoabsoprtion (UV-Vis) spectroscopy, Hall, resistivity and magnetoresistance measurements, X-ray photo electron spectroscopy (XPES) and secondary ion mass spectrometry (SIMS) to understand the e_ects of defects and disorder on the electrical and optical properties of doped ZnO thin films.

Publications

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3. Magnetic and dielectric behaviour in $YMn_{1-x}Fe_xO_3$ ($x \leq 0.5$)Neetika Sharma, A. Das, S. K. Mishra, C. L. Prajapat, M. R. Singh, and S. S. MeenaJ. Appl. Phys.115, 213911 (2014).
4. Phase separated behavior in Yttrium doped $CaMnO_3$Neetika Sharma, A. Das, C. L. Prajapat, Amit Kumar, and M. R. SinghMater. Res. Bull. 77, 284 (2016).
5. Effect of rare-earth dopants on the magnetic ordering of frustrated h-$YMnO_3$Neetika Sharma, A. Das, C. L. Prajapat, and M. R. SinghJ. Magn. Magn. Mater. (doi/ 10.1016/j.jmmm.2016.07.043).

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5. Magnetic and Optical properties of Fe doped crednerite $CuMnO_2$ K.K. Shukla, P. Shahi, Gopal S, A. Kumar, A. K. Ghosh, Ripandeep Singh, Neetika Sharma, A. Das, A. K. Sinha, Amish G. Joshi, A. K. Nigam, and Sandip Chatterjee RSC Adv. 5, 83504 (2015).

141. Name : **Abira Ganguly**
Enrolment No. : LIFE09201004025
Date of Award of degree : 13.12.16
Constituent Institute : Tata Memorial Centre
Title : “Size and Shape Control Mechanism of Nucleus”

Abstract

Organelle size and shape inside a cell is a basic fundamental cell biological interest to study. Altered organelle size and shape is always associated with some clinical aspects. “Karyoplasmic ratio” (the ratio of the nuclear volume to cell volume) remains roughly constant in cells with widely different DNA contents, ranging from single-cell eukaryote to mammalian cells. It is tempting to speculate that there is a tight regulation of nuclear size and shape in normal cell & that regulation is disrupted in case of cancer cells. The current understanding of the size and shape control mechanism of the largest organelle Nucleus is in its infancy. In the present study, two model organisms are studied to understand nucleus size and shape control mechanism. The candidate very well demonstrated alteration of both N/C ratio and size of nucleolus in different transformed cell lines compared to the immortalized cell lines of same tissue origin. Present concepts rely on nuclear size is determined by a limiting soluble component that originates in the cytoplasm and is transported to the nucleus. If this is true, then nuclear import/export would be expected to play a role in determining nuclear size. In this study it has been showed that perturbation of nucleo cytoplasmic transport can alter both N/C ratio and nucleolus size and number in immortalized cells. However, this increased N/C ratio could not change the invasion potential further of the same immortalized cells. Using an in vitro assay system, it has been demonstrated that cytosolic factors control size of nucleolus. In mammalian system, communication between nucleus and cytoplasm is very important to maintain the N/C ratio and nucleolus size in immortalized cells. In yeast system, using an unbiased approach, motor proteins (Kar3, Cin8) and pre mRNA splicing protein (Prp45) are found to control nuclear size and shape. In motor proteins Kar3, Cin8 and pre mRNA splicing protein Prp45 1-169, nuclear shape is altered in all stages of cell cycle. This study indicates that prp45 is one of the important gene that controls nuclear shape as well as sub nuclear domain like chromatin unlike Kar3 and Cin8 null mutants. In yeast, nucleus size and shape alteration phenotype can be achieved through many different genes or pathways. Alteration in nuclear surface area or volume does not necessarily alter the chromatin inside the nucleus always. .This very informative piece of work uses both human cell lines and budding yeast to generate extremely interesting data that will be valued highly in the community for not only its novel insights but also for its systematic and measured approach.

Publications

Journal

1. Febs Letters, Ganguly A, Bhattacherjee C, Bhave M, Kailaje V, Sengupta I, Jain B, Rangarajan A and Bhattacharyya D. Perturbation of nucleolcytoplasmic transport affect the size of nucleus and nucleolus. Febs Letters, Mar;590(5):631-43; PMID:26813731
2. To be submitted: Ganguly A. Bhattacharyya D. Nuclear kinesins Kar3, Cin8 and splicing protein prp45 ts mutants control nuclear shape and size in budding yeast Sacharomycescerevisiae (Manuscript under preparation)

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1. “7th Bangalore Microscopy course”, at NCBS, Bangalore, India in September 2015[Poster presentation: Attenuation of Nuclear import Affects Nucleus and Nucleolus Size in Human cells]
2. “18th International Microscopy Congress’’, at Prague, Czech Republic in September 2014 [Poster presentation: Nucleus Size and Shape Mystery]

3. "The All India Cell Biology Conference on Cell Dynamics and Cell Fate", at inSTEM-Bangalore, India in December, 2013 [Stage Presentation: Study to investigate nuclear size control mechanism]
4. “Society for Biological Chemists’’ at CIMAP-Lucknow, India in November 2011 [Poster presentation: To develop an assay system to study the Size and Shape control mechanism of Nucleus]

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1. Bhattacharjya S#, Roy KS#, Ganguly A, Sarkar S, Panda CK, Bhattacharyya D, Bhattacharyya NP, RoychoudhuryS. Inhibition of nucleoporin member Nup214 expression by miR-133b perturbs mitotic timing and leads to cell death. Mol Cancer. 2015 Feb 15;14(1):42. PMID: 25743594 .
2. Nath S#, Chowdhury A#, Dey S, Roychoudhury A, Ganguly A, Bhattacharyya D, Roychoudhury S. Deregulation of Rb-E2F1 axis causes chromosomal instability by engaging the transactivation function of Cdc20-anaphase-promoting complex/cyclosome. Mol Cell Biol. 2015 Jan;35(2):356-69. PMID: 25368385
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142. Name : **Abhay Gusain**
Enrolment No. : ENGG01201104015
Date of Award of degree : 22.12.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Development Of Organic Solar Cells And Their Performance Characterization.

Abstract

Organic solar cells based on conducting polymers offer multiple advantages like low weight, flexibility, low manufacturing costs, ease of integration with other products, low environmental impact during manufacturing and operations and short energy payback times. The present thesis aims at the development of the polymer solar cells based on conducting polymers - poly[N- 9'-heptadecanyl-2,7-carbazole-alt-5,5-(4,7-di-2-thienyl-2',1',3'-benzothiadiazole] (PCDTBT) and poly (3-hexylthiophene- 2,5–diyl) (P3HT). In particular, the origin of the S-kinks, an implication of the inefficient charge transfer in the bulk of the device, has been investigated and correlated effectively with the reduced efficiency of the solar cells. The origin of S-kinks has been correlated to the electron accumulation at the interfaces between the hole transport layer (HTL) and the active layer (PCDTBT:PCBM). Additionally, the improvement in the efficiency has been achieved by adopting two novel approaches – application of the solvent annealing for the improvement in the charge transfer across the interfaces and incorporation of graphene in the active layer for improvement in the charge transfer in the bulk of the devices. The solvent annealing (using Tetrahydrofuran –THF) improves the quality of the interfaces and thus reduces the electron density at these interfaces. The addition of graphene nanosheets in the active layer (P3HT:PCBM) showed a π-π interaction between the graphene and PCBM as confirmed from the shift in the onset of the reduction potential of PCBM from -0.56 V to -0.69 V. Such interaction causes an increase in the LUMO of PCBM, thereby leading to an increase in the open circuit voltage from 0.67 V to 0.76 V. In case of P3HT:PCBM solar cells, the overall improvement in the efficiency from 1.25% to 2.51% was achieved. While for PCDTBT:PCBM solar cells an efficiency improvement from 1.5% to 3.7% has been achieved. Thus, the study of the interface in particular observation of S-kinks has been beneficial for the improvement in the efficiency of the solar cells.

Publications

Journal

1. Electron density profile at the interfaces of bulk heterojunction solar cells and its implication on the S-kink, Abhay Gusain, S. Singh,A.K. Chauhan, V. Saxena, P. Jha, P.Veerender, A. Singh, P. V.Varde, SaibalBasu, D.K. Aswal and S.K. Gupta, *Chem. Phys. Lett.* 646, 6–11 (2016). (Thesis work)
2. Flexible NO gas sensor based on conducting polymer poly[*N*-9 -heptadecanyl-2,7-carbazole-alt-5,5-(4 ,7 -di-2-thienyl-2 ,1 ,3 -benzothiadiazole)] (PCDTBT), Abhay Gusain, Nirav Joshi,P. V. Varde, D.K. Aswal, *Sens. Actuators B Chem.* , 239, 734–745, (2017). (Thesis work)
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9. Free-standing polypyrrole films as substrate-free and Pt-free counter electrodes for quasi-solid dye-sensitized solar cells, P. Veerender, V.Saxena, P. Jha, S.P. Koiry, Abhay Gusain, S. Samanta, A.K. Chauhan, D.K. Aswal, S.K. Gupta, *Org. Electron.* 13(12), 3032-3039 (2012).
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11. Probing the annealing induced molecular ordering in bulk heterojunction polymer solar cells using in-situ Raman spectroscopy, P Veerender, V.Saxena, A.K. Chauhan, S.P.Koiry, P.Jha, Abhay Gusain, S. Choudhury, D.K.Aswal, S.K. Gupta, *Sol. Energ. Mat. Sol. Cells,*120, 526-535 (2013).

143. Name : **Rajeev Kumar**
Enrolment No. : PHYS01201004014
Date of Award of degree : 22.12.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Measurement of reactivity in sub-critical reactors using neutron noise methods.

Abstract

The research work carried out addresses problems associated with sub-critical reactivity measurement using noise methods, in view of the importance of such measurements to Accelerator Driven Systems (ADS). The main findings of the thesis are as follows.The statistical characteristics of accelerator based neutron sources are expected to be different from that of Poisson sources. Considerable amount of theoretical work has been done in the past at BARC and elsewhere to understand the implications of this difference in interpreting ADS noise. An experiment carried on an accelerator based D-T neutron source showed that the noise descriptors studied have characteristics that are different from that of a Poisson source.Heavy water moderated sub critical reactors are also being studied as possible candidates for ADS. Measurement of reactivity using noise methods is more involved in heavy water reactors in comparison with light water/fast reactor due to the significant contribution of delayed neutrons. The thesis presents reactivity measurements at different sub-criticality levels in a heavy water reactor. Thus it extends the scope of noise methods to heavy water moderated systems. Space dependent effects introduce large errors in the measurement reactivity by noise methods in deep sub-critical system. A method for mitigating such effects was demonstrated experimentally by carrying out measurement of the reactivity in a deep sub-critical system (k_{eff}~0.9). An important component of the work has been the development of a time stamping data acquisition system for noise studies. The work done is useful in context of the ongoing R&D in Accelerator Driven Systems.

Publications

Journal

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144. Name : **Poonam Sadhu Kakade**
Enrolment No. : LIFE09201004006
Date of Award of degree : 22.12.16
Constituent Institute : Tata Memorial Centre
Title : Role Of Glycosylation In Regulating Keratin 8/18 Functions.

Abstract

Keratins are intermediate filament proteins predominantly expressed in epithelial cells. Keratins 8/18 (K8/18) pair forms a major intermediate filament network in simple epithelia. It is post translationally modified with phosphate and O-GlcNAc moiety at multiple serine residues. There are three *O*-GlcNAcylation (Ser29, Ser30, and Ser48) and two phosphorylation (Ser33 and Ser52) sites on K18,which are well characterized. Both these dynamic modifications have been reported to increase K18 solubility and regulate their filament organization. However, investigation of specific O-GlcNAcylation site responsible for regulation of functional properties of K18 has not yet been done. In this report, we investigated the site-specific interplay between O-GlcnAcylation and phosphorylation in regulating the functional properties of K18, like solubility, stability and filament organization. An immortalized hepatocyte cell line (HHL-17) stably expressing site-specific single, double, and triple *O*-GlcNAc and phosphomutants of K18 were used to identify the site(s) critical for regulating these functions. Keratin 18 mutation of *O*-GlcNAcylation at Ser30 (K18-S30A) exhibited reduced phosphorylation induced solubility, increased stability, defective filament architecture, and slower migration. Interestingly, K18-S30A mutants also showed loss of phosphorylation at Ser33, a modification known to regulate the solubility of K18. Further to this, the K18 phosphomutant (K18-S33A) mimicked K18-S30A in its stability, filament organization, and cell migration. These results indicate that *O*-GlcNAcylation at Ser30 promotes phosphorylation at Ser33 to regulate the functional properties of K18 and also impact cellular processes like migration. *O*-GlcNAcylation and phosphorylation on the same or adjacent sites on most proteins antagonize each other in regulating protein functions. Here we report a novel, positive interplay between *O*-GlcNAcylation and phosphorylation at adjacent sites on K18 to regulate its fundamental properties.

Publications

Journal

1. Functional implications of O-GlcNAcylation dependent phosphorylation at proximal site on keratin 18. Kakade PS, Budnar S, Kalraiya RD, Vaidya MM,J Biol Chem. 2016 Apr 8. pii: jbc.M116.728717.

Conferences attended:

1. Presented a poster titled, the crosstalk between O-linked β-n-acetylglucosamine (O-GlcNAcylation)and phosphorylation of keratin 18 regulate its functional properties andcellular processes, at '2015 cell biology annual meeting' organized by American Society forCell Biology (ASCB) at San Diego convention Centre, California, USA (December, 2015).
2. Oral presentation titled, 'O-linked β-N-acetylglucosamine (O-GlcNAcylation) andphosphorylation crosstalk on keratin 18 regulates its stability and filament organization', at"Molecular Pathways to Therapeutics: Paradigms and Challenges in Oncology",Carcinogenesis 2015, International conference organized by Carcinogenesis Foundation, USAand TMC-ACTREC, India at, TMC-ACTREC, Navi Mumbai (February 2015).

3. Presented poster titled, ‘Understanding the role of O-GlcNAcylation of Keratin 18 inregulation of its critical properties and functions’ at ‘National Conference on “Glycobiology ofCancer; Lectins as tools and Targets” organised by Karnatak University, Dharwad, Karnataka,India (November, 2013)
4. Presented poster titled, ‘Role of O-GlcNAcylation in regulating keratin 8/18 properties’ at ’31Annual Convention Indian Association for Cancer Research 2012’ organized by TMCACTREC,Navi Mumbai, India. (February, 2012).

Others (Awards during the tenure):

1. Best poster award for ‘Understanding the role of O-GlcNAcylation of Keratin 18 inregulation of its critical properties and functions’ at ‘National Conference on “Glycobiology ofCancer; Lectins as tools and Targets” organised by Karnatak University, Dharwad, Karnataka,India (November, 2013)

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145. Name : **Shaikh Sazim**
Enrolment No. : PHYS07201004009
Date of Award of degree : 22.12.16
Constituent Institute : Institute of Physics,
Title : Quantum Correlations in Multiparticle Systems and Its Applications.

Abstract

Characterization of quantum correlations in multiparticle systems is of great interest due to its potential application in many quantum information processing tasks. It has importance in foundational aspects of quantum information science also. Out of different types of correlations, we focus on the quantum entanglement and Quantum Correlations that go beyond Entanglement (QCbE). Till date there exist no unique characterization method for quantum enatanglement and QCbE in multiparticle systems. We propose a detection method of entanglement in higher dimensional systems using the modified form of quantum covariance. Then we show that quantum discord may capture local as wel as nonlocal quantumness. Here, by local quantumness we mean local superposition (single particle) in a system of more than one particles. If this superposition can be masked by writting down the state in a different decomposition --- then the state has no local quantumness in it. The nonlocal superposition is the superposition of the states of two or more particles. We have also extended this analysis for more than two particle systems. We generalize the notion of quantum discord, using multivariate mutual information, to characterize the quantum properties of a multiparticle system. This new measure, called dissension, is a set of numbers -- quantumness vector. There are a number of different possible generalizations. We consider two of them. The Track-I generalization is discord type, while the Track-II generalization is based on all possible measurements. We give expressions for these generalizations for n-qubit systems, and explore some of their properties. We also consider a set of three-qubit and four-qubit states to illustrate the usefulness of the dissension vectors. In particular, we showed that different class of states can be characterized using dissension vectors. To give physical meaning to quantum correlations, we consider some exixting protocols like quantum teleportation, superdense coding, broadcasting etc. We used the concurrence monotones and developed some hierarchy of inequality relations by which one can infer

whether a two-qudit state is useful for teleportation. We have also considered a swapping network and analysed the entanglement between the nodes. Here, we considered quantum teleportation where a sender wants to send the quantum message through the network to a receiver and superdense coding where a sender wants to send the classical information to a receiver. Our results reflect that the entanglement between nodes of the network determines how much classical and quantum information one can send. Then, we have investigated the phenomenon of broadcasting of quantum correlations. We have shown that using any kind of local and nonlocal universal or state dependent cloning machines, the optimal broadcasting of QCbE is impossible and thus it indicates that the entanglement and QCbE are two distinct notions of correlations in quantum states. Also, we showed that the better we clone (delete) a state, the more difficult it will be to bring the state back to its original form by the process of deleting (cloning). This fact was demonstrated by introducing some complementarity relation between the correlations generated during the process.

Publications

Journal

1. "A Study of Teleportation and Super Dense Coding Capacity in Remote Entanglement Distribution" by Sk Sazim and I. Chakrabarty (Journal: *Euro. Phys. J. D 67,174 [8 pages] (2013)*).
2. "Quantification of Entanglement of teleportation in Arbitrary Dimensions"by Sk Sazim, Satyabrata Adhikari, Subhashish Banerjee, and Tanumoy Pramanik (Journal: *Quantum Information Processing 13, 863 – 880 (2014)*).
3. "Complementarity of Quantum Correlation in Cloning and Deleting ofQuantum State" by Sk Sazim, Indranil Chakrabarty, Annewsa Datta, and Arun K. Pati (Journal: *Phys. Rev. A 91, 062311 [11 pages] (2015)*).
4. "Retrieving and Routing Quantum Information in a Quantum Network" bySk Sazim, Indranil Chakrabarty, Chiranjeevi Vanarasa, and Kannan Srinathan (Journal: *Quantum Information Processing 14, 4651 – 4664 (2015)*).
5. "Quantum Coherence Sets The Quantum Speed Limit For Mixed States",Debasis Mondal, Chandan Datta, and Sk Sazim (Journal: *Phys. Lett. A 380, 689 – 695 (2016)*).
6. "Broadcasting of Quantum Correlations: Possibilities & Impossibilities"by Sourav Chatterjee, Sk Sazim, and Indranil Chakrabarty (Journal: *Phys. Rev. A 93, 042309 [13 pages] (2016)*).
7. "Quantum Discord has local and nonlocal quantumness" by Pankaj Agrawal, Indranil Chakrabarty, Sk Sazim, and Arun K. Pati (Journal: *Int. J. of Quantum Inform. 14, 1640034 [13 pages] (2016)*).

Communicated:

1. "Quantum mutual information and dissension vectors for multiqubit systems" by Sk Sazim and Pankaj Agrawal.

146. Name : **Biswajyoti Saha**
Enrolment No. : MATH10201204002
Date of Award of degree : 22.12.16
Constituent Institute : Institute of Mathematical Sciences,
Title : On the Analytic Continuation of Multiple Dirichlet Series and their Singularities

Abstract

For an integer $r \geq 1$, consider the open subset U_r of $\mathbb{C}^r$:

$$U_r := \{(s_1, \ldots, s_r) \in \mathbb{C}^r \ : \ \Re(s_1 + \cdots + s_i) > i \ \text{ for all } \ 1 \leq i \leq r\}.$$

The multiple zeta function of depth r, denoted by $\zeta_r(s_1, \ldots, s_r)$, is a function on U_r defined by

$$\zeta_r(s_1, \ldots, s_r) := \sum_{n_1 > \cdots > n_r > 0} n_1^{-s_1} \cdots n_r^{-s_r}.$$

The analytic continuation of multiple zeta functions was first established by Zhao and the exact set of singularities was identified by Akiyama, Egami and Tanigawa. After this Akiyama and Ishikawa introduced the notion of multiple Hurwitz zeta functions and multiple Dirichlet L-functions.

Let $r \geq 1$ be an integer, $\alpha_1, \ldots, \alpha_r \in [0, 1)$ and $\chi_1, \ldots, \chi_r$ be Dirichlet characters of any modulus. The multiple Hurwitz zeta function of depth r is denoted by $\zeta_r(s_1, \ldots, s_r;\ \alpha_1, \ldots, \alpha_r)$ and defined by the following convergent series in U_r:

$$\zeta_r(s_1, \ldots, s_r;\ \alpha_1, \ldots, \alpha_r) := \sum_{n_1 > \cdots > n_r > 0} (n_1 + \alpha_1)^{-s_1} \cdots (n_r + \alpha_r)^{-s_r},$$

and the multiple Dirichlet L-function of depth r is denoted by $L_r(s_1, \ldots, s_r;\ \chi_1, \ldots, \chi_r)$ and defined by the following convergent series in U_r:

$$L_r(s_1, \ldots, s_r;\ \chi_1, \ldots, \chi_r) := \sum_{n_1 > \cdots > n_r > 0} \frac{\chi_1(n_1) \cdots \chi_r(n_r)}{n_1^{s_1} \cdots n_r^{s_r}}.$$

Till date, we did not have precise information about the exact set of singularities of the multiple Hurwitz zeta functions and the multiple Dirichlet L-functions. Major part of this thesis is devoted to study these yet to be resolved problems.

Publications

Journal

1. "An elementary approach to the meromorphic continuation of some classical Dirichlet series", Biswajyoti Saha (to appear in Proc. Indian Acad. Sci. Math. Sci.).

2. "Analytic properties of multiple zeta functions and certain weighted variants, an elementaryapproach", Jay Mehta, Biswajyoti Saha and G.K. Viswanadham, J. Number Theory 168(2016), 487{508.

3. "Multiple Lerch zeta functions and an idea of Ramanujan", Sanoli Gun and Biswajyoti Saha(submitted, arXiv:1510.05835).

4. "Multiple Dirichlet series associated to additive and Dirichlet characters", Biswajyoti Saha(submitted).

Others

1. “Multiple Lerch zeta functions and an idea of Ramanujan”, Sanoli Gun and Biswajyoti Saha (submitted, arXiv: 1510.05835).
2. “Multiple Dirichlet series associated to additive and Dirichlet characters", BiswajyotiSaha (submitted).

147. Name : **Dushyant Kumar Sharma**
Enrolment No. : ENGG06201204001
Date of Award of degree : 22.12.16
Constituent Institute : Institute For Plasma Research,
Title : Slow Wave Characteristics Of Metamaterial Loaded Helical Guide.

Abstract

Slow Wave is an emerging area of research which promises many potential applications in the field of Optical Communication Network (OCN) [1-3], Microwave Photonics (MWP) [4] and Tele communication Network. In order to realize OCN architecture the Optical Data Packet Switching (ODPS) is highly desirable [1]. For ODPS, it is necessary to synchronize incoming data packets and regulate data traffic at network nodes or to implement congestion and contention resolution in the core routers [1]. Nowadays, electrical router performs these operations through large banks of Static Random Access Memory (SRAM). In OCN architecture this activity will be performed by optical buffers and memories. The mechanism of slow wave is vital for the development such devices. This thesis work is devoted to analyze the slow wave behavior of helical waveguide when its characteristics (structure induced dispersion) are superimposed with metamaterial properties (material induced dispersion). Different configurations of helical waveguide embedded with metamaterial medium are investigated and discussed. Significant amount of phase velocity reduction has been achieved in comparison to normal helix waveguide when it is in free space or loaded with normal dielectric column. The waveguide supports Hybrid (HE) mode propagation and possesses characteristics of Backward Wave (BW) mode, Forward Wave (FW) mode, zero-group velocity and mode-degeneracy. The large value of effective index of BW mode and mode-degeneracy mechanism leads to slowing and trapping of Electromagnetic (EM) wave. We, also, report that helical waveguide physical dimensions mainly radius and pitch angle act as tuning tools to control the phase velocity.

Publications

Journal

1. Propagation Characteristics of Extermently Anisotropic Metamaterial Loaded Helical Guide, D. K. Sharma and S. K. Pathak, Optics Express (Accepted).
2. Slowing and Stopping of Wave in Dispersive Metamaterial Loaded Helical Guide, D. K. Sharma and S. K. Pathak, Optics Express, Vol. 24, 2687-2700, 2016.
3. ENG Cladded Metamaterial Loaded Helical Guide for Optoelectronics Applications, D. K. Sharma and S. K. Pathak, Journal of Electromagnetic wave and Application (Taylor & Francis), Vol. 29, 2501-2511, 2015.
4. Ultra Slow EM Wave Propagation Characteristics of Left-Handed Material Loaded Helical Guide, D. K. Sharma and S. K. Pathak, Progress In Electromagnetics Research M (EMW Publishing USA), Vol. 35, 11-19, 2014.
5. Experimental analysis of novel FF-shaped metamaterial, D. K. Sharma and S. K. Pathak, IEEE Microwave and Components Letters (submitted).
6. Cross polarization converter formed by four F-shaped chiral metamaterial, D. K. Sharma and S. K. Pathak, IEEE Microwave and Components Letters (to be submitted).

Conferences

1. Dispersion Characteristics of Metamaterial Loaded Helical Guide, Dushyant K. Sharma and Surya K. Pathak, IEEE International Conference on Microwave and Photonics, ISM, Dhanbad, 2013.
2. Enhanced Slow Wave through Dispersive Metamaterial Loaded Helical Guide: Analytical Study and Design, Dushyant K. Sharma and Surya K. Pathak, OSA International Conference on Fibre Optics and Photonics, IIT, Kharagpura, 2014.
3. Enhanced Group Velocity Characteristics of a ENG Cladded Metamaterial Loaded Helical Guide, Dushyant K. Sharma and Surya K. Pathak, Progress In Electromagnetics Research Symposium, Prague, European Union, 2015.

4. Broadband Cross Polarization Converter Formed by Twisted F-Shaped Chiral Metamaterial, Dushyant K. Sharma and Surya K. Pathak, Progress In electromagnetic Research Symposium, Prague, European Union, 2015.

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148. Name : **Subrata Ghosh**
Enrolment No. : PHYS02201104005
Date of Award of degree : 22.12.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,,
Title : Vertical Graphene Nanosheets: Growth, Structure and Electrochemical Performance.

Abstract

Due to the unique geometry, high surface area, good electrical conductivity and open three-dimensional network, vertical graphene nanosheets (VGN) received strong momentum towards its wide range of applications. To utilize them in potential applications, a clear understanding of the growth mechanism and optimization of growth parameters to achieve desired morphology is highly essential. With this motivation, the present work is addressed towards synthesis and studies of VGN on various substrates and their application towards supercapacitor (SC) electrode.A systematic study on synthesis of VGN using electron cyclotron resonance - plasma enhanced chemical vapor deposition is carried out. The effect of growth time, feedstock gas composition, growth temperature, microwave power, distance from plasma source to substrate and role of substrates on the growth and structural properties of VGN are addressed. The experimental observations reveal that the morphology can be tuned from vertical to planar structure by changing the growth parameters. Further, direct correlation between XPS and Raman analysis in terms of vacancy-like defects is obtained. Based on the results from influence of feedstock gas compositions, a ternary field diagram clearly demorcating the region of VGN growth is established. A phenomenological four stage growth model is proposed and discussed, to substantiate the defect-induced nucleation and growth mechanism of VGN by invoking substrate-plasma interaction during growth. Formation of defects at early stage nucleation is found to dictate the morphology and structural quality of VGN.

Finally, the electrochemical performance of VGN of optimized morphology and suitable aqueouselectrolyte for its effective utilization as a SC electrode is investigated. To explore the capacitative behaviour under various aqueous electrolytes (Na_2SO_4, KOH, and H_2SO_4), the electrochemical investigation of VGN are carried out using three electrode system. An electrical equivalent circuit modeling is performed based on electrochemical impedance spectroscopy to elucidate the electrolyte-electrode interaction. H_2SO_4 is found to be a choice of electrolyte in terms of specific capacitance, cycle life, efficiency and time constant. Integration of VGN with transition metal oxides (TMO) is a promising approach to further enhance the capacitance of VGN. Due to the fast redox kinetics, less toxicity and less expensive, MnO_2 is chosen out of TMO and decorated on the surface of VGN. Apart from the enhancement in capacitance of the composite by five times, VGN is found to serve as an excellent mechanical backbone for the effective utilization of MnO_2 without any structural degradation. The observed results demonstrate that the VGN and its composites can be a potential candidate for SC applications.

Publications

Journal

1. Supercapacitive Vertical Graphene Nanosheets in Aqueous Electrolytes, Subrata Ghosh, Tom Mathews, Bhavana Gupta, A. Das, Nanda Gopala Krishna and M. Kamruddin. arXiv:1603.08320

2. A Route Towards Controlling the Morphology of Vertical Graphene Nanosheets, Subrata Ghosh, K. Ganesan, S. R. Polaki and M. Kamruddin. 2016, arXiv:1603.08322
3. MnO_2/Vertical Graphene Nanosheets as Active Materials for Energy Storage, Subrata Ghosh, Bhavana Gupta, K. Ganesan, A. Das, M. kamruddin, Sitaram Dash and A. K. Tyagi, *Mat. Today Proc.*, 2016 *3*, 1686-1692
4. Effect of Annealing on the Structural Properties of Vertical Graphene Nanosheets, Subrata Ghosh, K. Ganesan, S. R. Polaki, A. K. Sivadasan, M. Kamruddin and A. K. Tyagi, *Adv. Sc. Eng. Med.* 2016; *8*,146-149
5. Flipping Growth Orientation of Nanographitic Structures by Plasma Enhanced Chemical Vapor Deposition, Subrata Ghosh, K. Ganesan, S. R. Polaki, S. Ilango, S. Amrithapandian, S. Dhara, M. Kamruddin and A. K. Tyagi, *RSC Adv.* 2015, *5*, 91922-91931
6. Influence of Substrate on Nucleation and Growth of Vertical Graphene Nanosheets, Subrata Ghosh, K. Ganesan, S. R. Polaki, Tom Mathews, Sandip Dhara, M. Kamruddin and A. K. Tyagi, *Appl. Surf. Sc.* 2015, *349*, 576-581
7. Evolution and Defect Analysis of Vertical Graphene Nanosheets, Subrata Ghosh, K. Ganesan, Shyamal. R. Polaki, T. R. Ravindran, Nanda Gopala Krishna, M. Kamruddin and A. K. Tyagi *J. Raman Spectrosco.* 2014, *45*, 642-649 arXiv: 1402.2074v3

Not included in thesis

8. A Comparative Study on Defect Estimation using XPS and Raman Spectroscopy in Few Layer Nanographitic Structures. K. Ganesan, Subrata Ghosh, Nanda Gopala Krishna, S. Ilango, M Kamruddin, and A K Tyagi, *Phys. Chem. Chem. Phys*. 2016, 18, 22160-22167. arXiv: 1607.04482v1
9. Temperature and Pressure Dependent Raman Spectroscopic Studies and Thermal Conductivity of Vertical Graphene Nanosheets. K. K. Mishra, Subrata Ghosh, T. R. Ravindran, S. Amrithapandian, and M. Kamruddin, *J. Phys. Chem. C* 2016, DOI: 10.1021/acs.jpcc.6b08754
10. Vertical Graphene Nanosheets for Supercapacitor Application in Organic Electrolyte, Subrata Ghosh, Madhusmita Sahoo, T. Mathews and M. Kamruddin, (Submitted)
11. Heterogeneous Electron Transfer Properties of Vertical Graphene Nanosheets, Dale Brownson, Subrata Ghosh, C. E. Banks and M. Kamruddin, (Manuscript under preparation

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149. Name : **K. R. Rasmi**
Enrolment No. : CHEM02201004006
Date of Award of degree : 22.12.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,,
Title : Synthesis Of Noble Metal Nano Coatings On Titanium For Electrode Application.

Abstract

Title: Synthesis of Noble Metal Nano Coatings on Titanium for Electrode ApplicationThe present Ph.D. thesis contributes to the development of advanced high corrosion resistant noble metal nanostructured coatings on Ti for electrode applications. The noble nanoparticle coated electrodes studied in the thesis are Pt nanoparticle coated Ti, Pd nanoparticle coated Ti and Pt nanoparticle loaded TiO_2 nanotube array. A two step reduction process involving seed mediated hydrothermal reduction method was adopted for the synthesis of nanoparticle coating. This method generated a uniform and highly dispersed nanoparticle coating on Ti which is highly essential for the application in severe corrosive medium. The seed particles acted as sites with less activation energy for further nucleation and growth of metal nanoparticle during hydrothermal reduction.The physical and electrochemical properties of the as developed electrode were investigated for the application in severe corrosive medium. The size, shape, crystal structure, oxidation state and electrocatalytic activity of the noble metal nanoparticles in the coating was studied in detail. From the cross hatch tape test, linear scratch test and electrochemical oxidation of Ce in 11.5 M nitric acid studies, it was observed that Pt nanoparticle coated Ti and Pt nanoparticle loaded TiO_2 nanotube array were superior to Pd nanoparticle coated Ti. Further, both Pt nanoparticle coated Ti and TiO_2 nanotube array were selected for long term durability testing and electrode life assessment study in Ce containing 11.5M nitric acid at 9mA/cm^{2}current density. The surface of both electrodes was tested using Scanning electron microscopy (SEM) and elemental mapping after 1000 h. From the post characterization studies, it was observed that Pt nanoparticles were intact in Pt nanoparticle loaded TiO_2nanotube array electrode and it showed excellent corrosion resistance than Pt nanoparticle coated Ti. This indicates that the stability of Pt coating is much better on TiO_2 nanotube array than Ti substrate. The higher corrosion resistance and strong interactions with metal nanoparticle catalyst of TiO_2 nanotube array substrate could prevent the agglomeration of metal particles resulting in better adhesion and coating stability. The enhanced surface area provided by TiO_2 nanotube array was responsible for more particle dispersion and high coating stability. The life assessment of both electrodes was carried out and Pt nanoparticle coated TiO_2 nanotube array electrode was assessed to be 1728 h and that of Pt nanoparticle coated Ti was 1152 h at a current density of 9mA/cm2 in Ce containing 11.5M nitric acid.

Publications

Journal

1. "Synthesis and Characterization of Nano Structured Platinum Coated Titanium as Electrode Material", K. R. Rasmi, S. C. Vanithakumari, R. P. George and U. Kamachi Mudali, Journal of Materials Engineering and Performances, 2014, 23, 1673-1679.
2. "Nano Platinum Coated Titanium Electrode for Application in Severe Corrosive Medium", K. R. Rasmi, S. C. Vanithakumari, R. P. George, C. Mallika and U. Kamachi Mudali, Materials Chemistry and Physics, 2015, 151, 133-139.
3. "Nanoparticles of Pt loaded on vertically aligned TiO_2 nanotube bed: Synthesis and evaluation of electrocatalytic activity", K. R. Rasmi, S.C. Vanithakumari, R.P. George, C. Mallika, U. Kamachi Mudali, RSC Advances, 2015, 5, 108050-108057.
4. "Stability and Durability of Nano Pt Coated Titanium Electrode for Electrocatalytic Application", K. R. Rasmi, S. C. Vanithakumari, R. P. George, C. Mallika and U. Kamachi Mudali, Transactions of the Indian Institute of Metals (Accepted)
5. "Comparison of Nanoparticles Coated Electrode Properties and Long Term Durability Studies in Severe Corrosive Medium", K. R. Rasmi, S. C. Vanithakumari, R. P. George, C. Mallika and U. Kamachi Mudali, (to be communicated to Journal of Nuclear Materials)
6. "Pd nanoparticle coated Ti –Synthesis, characterization and its electrocatalytic activity Study", K. R. Rasmi, S. C. Vanithakumari, R. P. George, C. Mallika and U. Kamachi Mudali, (to be communicated to Applied Surface Science

Conferences:

1. K. R. Rasmi, S. C. Vanithakumari, R. P. George and U. Kamachi Mudali, "Active nano metal oxide coating for anti-biofouling". 5th Training Program on Paints and Coating, 13th-15th July, 2012 at Hotel Jayapuspam, Chennai.

2. K. R. Rasmi, S. C. Vanithakumari, R. P. George and U. Kamachi Mudali, “Studies to Optimize Electrodeposition of Pt Nanoparticle on Titanium”, National Symposium on Electrochemical Science &Technology, NSEST – 2012, 24th-25th August, 2012, Indian Institute of Science, Bengaluru.
3. K. R. Rasmi, S. C. Vanithakumari, R. P. George and U. Kamachi Mudali, “Active Nano Metal Oxide Coating for Bio-fouling Resistance”, International Conference on Corrosion (CORCON 2012), NACE India Section Goa, 26th-29th September, 2012, Goa.
4. K. R. Rasmi, S. C. Vanithakumari, R. P. George and U. Kamachi Mudali, “Synthesis, Characterization and Electrochemical Study of Titanium Electrodes Decorated with Pt Nanoparticles” Recent Trends in Material Chemistry-RTMC-2013, 25th-27th July, 2013 at VIT, Vellore.
5. K. R. Rasmi, S.C. Vanithakumari, R.P. George, U. Kamachi Mudali, "Effect of deposition parameters on the electrodeposition of platinum on titanium", paper presented at International Corrosion Prevention Symposium for Research Scholars, CORSYM-2013, 28th February-2nd March, 2013, Chennai.
6. K. R. Rasmi, S. C. Vanithakumari, R. P. George and U. Kamachi Mudali, Poster presentation at NIGIS South Zone Student Poster Session during Short Term Training Course on Corrosion and its Control on 30th-31st January, 2014 at SRM University, Tamil Nadu, India.
7. K. R. Rasmi, S. C. Vanithakumari, R. P. George and U. Kamachi Mudali, “Synthesis, Characterization and Application of Pt Nano Particle Coated Ti Electrode” CORSYM 2014, 20th - 21st February, 2014, at Indian Institute of Technology, MUMBAI.
8. K. R. Rasmi, S. C. Vanithakumari, R. P. George and U. Kamachi Mudali, “Synthesis and Characterisation of Electrocatalytically Active Platinum Nano Particles Deposited on Titanium" Poster presentation at 583rd Wilhelm und Else Heraeus Seminar on Electrochemical Surface Science”, 18th to 22nd January, 2015 at Physikzentrum Bad Honnef, Germany.
9. K. R. Rasmi, S. C. Vanithakumari, R. P. George and U. Kamachi Mudali, "Synthesis and Electrocatalytic Activity of Platinum Loaded TiO_2 Nanotube for Electrode Application in Severe Corrosive Medium", CORSYM 2015, 31st July-01st August, 2015 at IIT Madras, Chennai.
10. K. R. Rasmi, S. C. Vanithakumari, R. P. George, C. Mallika and U. Kamachi Mudali, "Long Term Evaluation of the Durability of Pt Nanoparticle Coated Titanium Electrode in Severe Corrosive Environment", International Corrosion Conference and Expo-CORCON 2015”, 19th-21st November, 2015 at Chennai Trade Center.

* * *

150. Name : **Varun Hassija**
Enrolment No. : CHEM02201004006
Date of Award of degree : 22.12.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,,
Title : Development And Application Of Probabilistic Safety Assessment Methodologies For Estimating Risk From Nuclear Power Plants.

Abstract

The present thesis is focused towards, (i) common cause failure analysis for engineered safety systems using alpha factors obtained by mapping technique, (ii) dynamic modelling of the scenarios with time dependent success criteria and (iii) development of an integrated approach to assess the risk from multi unit nuclear power plants sites with consideration of both external and internal hazards. In the first part of the research work, common cause failure analysis for engineered safety systems using alpha factors obtained by mapping technique is carried out. Here an approach described in NUREG/CR-5500 is extended in this study to derive plant specific coefficients for CCF analysis especially for high redundant systems. A critical comparison of

alpha factor method and beta factor method is also performed by taking insights from the case studies of engineered safety systems installed in existent nuclear power plants. In the second part of the research work "Markov Analysis for Time Dependent Success Criteria of Passive Decay Heat Removal System" is carried out. The approach described can be used to dynamically model the scenarios with time dependent success criteria in a comprehensive manner and to study various factors affecting the availability of such systems.Finally, in the last part of the research work "Integrated risk assessment for multi-unit NPP sites" is performed. Traditionally, a PSA is carried out to evaluate the risk associated with single unit NPP taking into account the defence in depth features and postulating combination of potential accident initiators for different hazards. At present, there exists no established approach or methodology to estimate the risk from a multi-unit nuclear power plant site due to internal and external hazards. Hence, there is an urgent need to evolve a methodology which can systematically assess the safety of the multi-unit site. In this work, a methodology is developed to address various issues at a multi-unit NPP site to estimate site risk.

Publications

Journal

1. Varun Hassija, C. Senthil Kumar, K. Velusamy, "A pragmatic approach to estimate alpha factors for common cause failure analysis", Annals of Nuclear Energy, Volume 63, January 2014, Pages 317-325.
2. Varun Hassija, C. Senthil Kumar, K. Velusamy. "Markov Analysis for Time Dependent Success Criteria of Passive Decay Heat Removal System", Annals of Nuclear Energy, Volume 72, October 2014, Pages 298-310.
3. Varun Hassija, C. Senthil Kumar, K. Velusamy, "Probabilistic safety assessment of multi-unit nuclear power plant sites – An integrated approach", Journal of Loss Prevention in the Process Industries, Volume 32, November 2014, Pages 52-62.
4. C. Senthil Kumar, Varun Hassija, K. Velusamy and V. Balasubramaniyan, "Integrated risk assessment for multi-unit NPP sites – A comparison" , Nuclear Engineering and Design, Volume 293, November 2015, Pages 53-62.

Conference Proceedings

1. Varun Hassija, C. Senthil Kumar, K. Velusamy. "Development in PSA methodology based on the lessons learnt from the Fukushima Nuclear Disaster", Second International Conference on Advances in Industrial Engineering Applications (ICAIEA 2014), Anna University, Chennai, 2014.
2. Varun Hassija, C. Senthil Kumar, K. Velusamy. "Common Cause Failure analysis for Engineered Safety Systems using alpha factors obtained by mapping technique", International Workshop on New Horizons in Nuclear Reactor Thermal Hydraulics and Safety (IW-NRTHS 2014), Mumbai, 2014.
3. C. Senthil Kumar, Varun Hassija, K. Velusamy. "Risk Assessment of Multi-Unit Nuclear Power Plant Sites Against External Hazards", International Workshop on New Horizons in Nuclear Reactor Thermal Hydraulics and Safety (IW-NRTHS 2014), Mumbai, 2014.
4. C. Senthil Kumar, Varun Hassija, V. Balasubramaniyan, A.John Arul, M. Prasad, V. Gopika, R. Nama, Rajee Guptan and P.V.Varde, "Risk Assessment of Multi-Unit Nuclear Power Plant Sites", International Workshop on Multi-Unit Probabilistic Safety Assessment (IW-MUPSA 2014), Ottawa, Canada, 2014.
5. Varun Hassija, C. Senthil Kumar, K. Velusamy. "A Comparative Risk Assessment for Sites with Single and Double Units", Advances in Reliability Maintenance and Safety - International Conference on Reliability Safety and Hazard Conference (ICRESH-ARMS 2015), Luleå University of Technology, Lulea, Sweden, 2015.

151. Name : **B. Sasi**
Enrolment No. : ENGG02200804020
Date of Award of degree : 22.12.16
Constituent Institute : Indira Gandhi Centre for Atomic Research,,
Title : Image Processing Approaches For Noise Reduction In Eddy Current Images.

Abstract

Nondestructive evaluation (NDE) plays an important role in ensuring structural integrity of engineering components through detection and sizing of flaws. It is very important to detect flaws in components at the early stages to prevent catastrophic failures. Eddy current (EC) NDE technique is simultaneously influenced by several variables such as surface roughness, variations in probe lift-off, variations in electrical conductivity and magnetic permeability and variations in geometry, apart from flaws. These variations produce large amplitude noise and thus, often mask information from shallow surface flaws as well as deep seated flaws. Although EC imaging is helpful, detection of shallow surface flaws in the presence of such composite noise is challenging. Removal of noise in EC images is time consuming, as it involves the use of several methods of processing depending on the sources of noise. The reported literature on processing of EC images, influenced by noise, is limited to handling one disturbing variable at a time. Information related to processing of composite noise in EC images is scarce in open literature. This demands development of image processing approaches for automated removal of noise in EC images while retaining maximum possible information related to flaws.This thesis presents the development of image processing approaches for noise reduction in EC images of surface flaws in AISI type 316 Stainless steels. It incorporates spatially adaptive noise filtering using multiresolution analysis by Discrete Wavelet Transform (DWT). It explores Independent Component Analysis (ICA) technique that involves separation of sources of noise based on their statistical independence.

Extensive studies have been carried out on the EC images acquired from plates, weld plates and thin walled tubes made of AISI type 316 stainless steels to develop the DWT and ICA based approaches. Performances of these approaches have been evaluated using Noise Reduction Percentage (NRP) and Signal to Noise Ratio (SNR). This thesis proposes a hybrid image processing approach by combining the advantage of the noise reduction ability of DWT based approach and the flaw retention ability of ICA based approach. A significant enhancement in flaw amplitude has been achieved by the proposed hybrid approach as compared to the individual processing approaches. The hybrid approach is found to be noise tolerant to variations in lift-off up to ≤1.5 mm.The efficacy of the proposed hybrid approach has been successfully demonstrated on EC images acquired at various frequencies (20 kHz, 75 kHz and 150 kHz) using probes of 3.0 mm, 5.0 mm and 20.0 mm diameter. The denoising capability of the proposed hybrid approach has been successfully validated on the influence of composite noise from variation in lift-off and wall thickness (geometrical variations) in thin wall SS tubes. The applicability of the proposed hybrid approach has been evaluated for enhancement of sub-surface flaws and natural crack. The hybrid approach proposed in this thesis has significantly enhanced the flaw detection sensitivity. It has also provided better insight into the existence of statistical dependency and utilization of dependency for enhanced effective separation of flaw information. The approach proposed in this thesis can be applied to EC images of flaws of varying orientation, width and depth and can be extended to other NDE images.

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1. B. Sasi, M.S. Ahamed Ali, C. Babu Rao and T. Jayakumar, "Effective de-noising and characterization of flaws in eddy current-NDE images, Int. Journal of Signal and Imaging System Engineering, Vol.7, No.3, pp. 236-251, 2014.
2. B. Sasi, Matteo Cacciola, C. Babu Rao, T. Jayakumar and Baldev Raj, "Hybrid signal processing approach for enhanced detection of flaws in eddy current NDE", Research in NDE, Vol.24, No.1, pp. 51-61, 2013.

3. B. Sasi, Matteo Cacciola, Lalita Udpa, B.P.C. Rao, T. Jayakumar and Baldev Raj, “Development of image fusion methodology for EC images using discrete wavelet transform”, NDT & E International, Vol.51, pp. 51-57, 2012.
4. B. Sasi, B.P.C. Rao, T. Jayakumar and Baldev Raj, “Wavelet transform based de-noising method for processing eddy current signals”, Research in NDE, Vol.21, No.3, pp.157-170, 2010.

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1. B. Sasi, C. Babu Rao, B.P.C. Rao, and T. Jayakumar, “Development of an automated image processing approach for quality control of component Eddy Current Instrument for Non-destructive Evaluation”, presented during 12th International Conference on Quality Control by Artificial Vision, June, 2015.
2. B. Sasi, B.P.C. Rao, C. Babu Rao and T. Jayakumar, “Enhancement on defect detection in Eddy Current NDE using hybrid image processing approach”, presented during conference on Review of progress in Quantitative Nondestructive Evaluation, Denver, July, 2012

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152. Name : **Utkarsh Mishra**
Enrolment No. : PHYS08201004005
Date of Award of degree : 26.12.16
Constituent Institute : Harish-Chandra Research Institute
Title : Dynamics Of Quantum Correlations In Clean And Disordered Many-Particle Systems.

Abstract

Quantum correlations are indispensable resource in quantum information theory and have been proven to be useful in realizing many quantum information protocols such as quantum dense coding, quantum teleportation, quantum cryptography, and one-way quantum computation. It has been observed that some of these protocols may be realized in many-body quantum systems, e.g., in spin-chain, optical lattices etc. Also, it has been seen that quantum correlations can be a tool in dealing with quantum many-body systems. These investigations have highlighted the importance of studying the behavior of quantum correlations in many-body systems. In the proposed thesis, we investigate the properties of quantum correlations in paradigmatic clean and disordered quantum many-body systems. The content of the proposed thesis is divided in to two parts. In the first part of the thesis, we identify a macroscopic quantum superposition state (Schroedinger cat state) that is resistant to particle loss and all types of decoherence. The resilience to particle loss and noise is better than that in the existing cat states in the literature. In the second part of the thesis, we discuss the behavior of quantum correlations in many-body systems described by XYZ (Heisenberg) Hamiltonians, both in “clean” and “disordered” cases. The discussion is in two separate but related contexts. In the first, we consider a clean system, which is quenched to zero at the initial instant. The ensuing dynamics is then investigated and we find that the system supports an ergodic-nonergodic transition. We observe that while bipartite entanglement remains always ergodic, independent of the choice of the parameters of the Hamiltonian, quantum discord between two sites show a transition from being non-ergodic for a certain values of the parameters to being ergodic for others. This result has been observed for the above model in 1D, ladder and 2D lattice. In the second “context” of the second part, we consider quenched disordered quantum spin-models and investigate their quenched averaged quantum correlations. We find that quenched disordered couplings in a quantum Heisenberg spin glass model can constructively interfere to enhance genuine multipartite entanglement in the ground state. We find here that such constructive interference is absent in the case of bipartite entanglement.

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1. Quantum superposition in composite systems of microscopic and macroscopic parts resistant to particle loss and local decoherence, Utkarsh Mishra, Aditi Sen (De), and Ujjwal Sen, *Phys. Rev. A*, 2013, *87*, 052117.
2. Tuning interaction strength leads to ergodic-nonergodic transition of quantum correlations in anisotropic Heisenberg spin model, Utkarsh Mishra, R. Prabhu, Aditi Sen (De), and Ujjwal Sen, *Phys. Rev. A*, 2013, *87*, 052318.
3. Local decoherence-resistant quantum states of large systems, Utkarsh Mishra, Aditi Sen (De), and Ujjwal Sen, *Phys. Lett. A*, 2015, *379*, 261-271.
4. Survival of time-evolved quantum correlations depends on whether quenching is across critical point in XY spin chain, Utkarsh Mishra, Debraj Rakshit, and R. Prabhu, *Phys. Rev. A*, 2016, *93*, 042322.
5. Constructive Interference between disordered couplings enhances multipartite entanglement in quantum Heisenberg spin glass models, point in XY spin chain, Utkarsh Mishra, Debraj Rakshit, and R. Prabhu , Aditi Sen (De), and Ujjwal Sen, *New J. Phys*., 2016, *18*, 083044.

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153. Name : **Amit Chandrakar**
Enrolment No. : ENGG01201104008
Date of Award of degree : 26.12.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Passive System Reliability Analysis.

Abstract

Passive safety systems are the systems which work based on natural laws, properties of materials, internally stored energy, etc. Deployment of passive systems in nuclear reactors provides several benefits, such as: avoidance of dependency on active components; such systems are simple and easy to build, operate and maintain. One of the issues with the passive systems is quantification of functional reliability for these systems during normal operation, transients including accidental conditions. The objective of this thesis was to develop a new methodology for the reliability analysis of passive systems, which addresses the following unresolved issues in reliability estimation of passive systems:

a. Treatment of dynamic failure characteristics of components

b. Quantification of functional failure probability of components of passive systems

c. Treatment of independent process parameters variations

d. Treatment of model uncertainties

In view of the unresolved issues associated with the currently available methodologies of passive system reliability analysis, a methodology called APSRA+ has been developed in this thesis to address the unresolved issues. APSRA+ provides an integrated dynamic reliability methodology for the treatment of dynamic failure characteristics of components such as multi-state failure, fault increment and time dependent failure rate of components of passive systems. Since there is serious lack of the database for multi-state failure probability of the mechanical components of passive system like valves, an experimental facility of a passive system consisting of three control valves was built and a series of experiments were performed to quantify the functional failure probability of these valves. From the experiments performed, the intermediate state

failure probabilities of valves were determined. APSRA+ has been applied to passive isolation condenser system (ICS) of Indian advanced reactor: Advanced Heavy Water Reactor (AHWR) as an example. Failure probability of ICS with respect to the reactor years has been estimated, which is of the order 1×10^{-10}. To treat variation of independent process parameters such as atmospheric temperature, which has significant effect on system performance and failure, the ARIMA model was adopted, which treats the variation of atmospheric temperature and predicts the probability of variation of this parameter.

Publications

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1. A. CHANDRAKAR, A. K. NAYAK and V. GOPIKA, “Development of methodology APSRA^{+} for passive system reliability analysis and its application to passive isolation condenser system of an advanced reactor,” Nuclear Technology; 194,2 (2016); http://dx.doi.org/ 10.13182/ NT15-80
2. A. CHANDRAKAR, A. K. NAYAK and V. GOPIKA, “Reliability analysis of process controlled systems considering dynamic failure of components,” Int. J. Syst. Assur. Eng. Management; 6, 2 (2014); http://dx.doi.org/10.1007/s13198-014-0248-z
3. A. K. NAYAK, A. CHANDRAKAR and V. GOPIKA, “A review: passive system reliability analysis – accomplishments and unresolved issues,” Front. Energy Res., 2,40 (2014); http://dx.doi.org/10.3389/fenrg.2014.00040.
4. A. CHANDRAKAR, A. K. NAYAK and V. GOPIKA, “Quantification of functional failure probability of a passive safety system,” SRESA Journal of Life Cycle Reliability and Safety Engineering (Accepted for publication).

Conferences:

1. Reliability Analysis of Process Controlled Systems Considering Dynamic Failure of Components. International Applied Reliability Symposium (ARS), September-2013
2. Passive System Reliability Analysis Challenges and a Step Towards Resolution. New Horizons in Nuclear Thermal Hydraulics and Safety, December, 2013.

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154. Name : **Lakshmi S. Mohan**
Enrolment No. : PHYS01200904008
Date of Award of degree : 26.12.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Precision measurement of neutrino oscillation parameters at INO ICAL

Abstract

The proposed India-based Neutrino Observatory will house a 50 kton magnetised detector for the detection of atmospheric neutrinos and determining the neutrino oscillation parameters in the 2–3 sector by studying the Earth matter effects on neutrino propagation. The main goal of the magnetised Iron Calorimeter detector (ICAL) is to determine the neutrino mass hierarchy; i.e, if the neutrino masses are ordered as m1 < m2 << m3 or m3 << m1 < m2. In addition ICAL can perform the precision measurement on the 2–3 mixing angle _23 and the mass squared difference |_m232(31)|. The channel ofinteraction of interest is the charged current interaction of _μ (¯_μ) with the iron target to produce μ−(μ+) and hadrons in the final state. The final states which are charged will be detected by the active detector elements resistive plate chambers interleaved with the iron layers. The X and Y pickup strips in each RPC give hit information along with the layer and timing information; i.e, (x, y, z, t) of the hit. The reconstruction of the final state particles are done using this hit information. GEANT4 based simulationstudies are done to study the propagation of various particles through ICAL and thus obtain the energy and direction of hadrons in ICAL. To reconstruct the energy of the hadron shower, the number of hits in it are counted and the energy is calibrated to the number of hits. The study of the energy resolution of hadrons as a funtion of plate thickness was also conducted for eleven different plate thicknesses including the default 5.6 cm of Fe plate in ICAL. Comparison of ICAL simulations with data and simulations of other experiments were also done. To characterise the effect of neutral pions on the hadron energy response the e/h ratio, which is the ratio of the electron response to hadron response of ICAL was calculated. For the reconstruction of hadron direction at ICAL the hit information along with the timing of the hits are used. This method called the "raw hit method" can be used to reconstruct hadrons from both charged current and neutral current interactions. For fixed energy single pions in the vertical direction cos _ = 0.9 the resolution is _ 9 when the reconstructed direction is fitted with a Gaussian. For multiple hadrons from neutrino interactions generated using NUANCE neutrino generator this is about _ 18 in the energy bin 1–2 GeV and _ 11 in the 14–15 GeV bin. The sensitivity studies to neutrino oscillation parameters in the 2–3 were done for 500 kton year exposure of ICAL. The _μ and ¯_μ events are binned separately in the observed bins of muon momentum and direction and hadron energy, (Eμ, cos _μ,E had) in the ranges 0.5–25 GeV, [-1, 1] and 0-15 GeV respectively. When only (Eμ, cos _μ) are used, it is called 2d binning and when (Eμ, cos _μ,E had) are used it is the 3D binning. In addition to extending the range of observed Eμ to 0.5–25 GeV, a constraint on the _μ/¯_μ flux ratio is imposed as a systematic in the analysis. These give a better precision on both sin2 _23 as well as |_m2 32| and also improves the hierarchy sensitivity of ICAL. For 500 kton year exposure of ICAL and 3D binning and with 11 pulls, the 1_ precisions on sin2 _23 and |_m23 2| are _ 9% and _ 2.5% respectively with normal hierarchy as the true hierarchy. For the same exposure, the masshierarchy sensitivity achievable with this combination when the true hierarchy is normal is __2 _ 8.5.

Publications

Journal

1. M.M. Devi, A. Ghosh, D. Kaur, S.M. Lakshmi, et al., "Hadron energy response ofthe Iron Calorimeter de- tector at the India-based Neutrino Observatory", JINST8, P11003, 2013 [arXiv:1304.5115 [physics.ins-det]].
2. S.M. Lakshmi, A. Ghosh, M.M. Devi, D. Kaur, et al., "Simulation studies ofhadron energy resolution as a function of iron plate thickness at INO-ICAL",JINST 9, T09003, 2014 [arXiv:1401.2779 [physics.ins-det]].

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1. M.M. Devi, S.M. Lakshmi, A. Dighe and D. Indumathi, "The physics reach ofICAL using hadron direction resolution", 2015.
2. S.M. Lakshmi, D. Indumathi, N. Sinha, "Probing sensitivities to atmosphericneutrino oscillation parameters by the addition of higher energies in muons andconstraining the neutrino-antineutrino flux ratio", 2015.

•Other publications

1. Lakshmi S Mohan : "Hadron energy response as a function of plate thickness andangular resolution of hadrons at the ICAL detector in INO", abstract, XX DAE-BRNS, High Energy Physics Symposium, January 13-18, 2013, Visva-Bharati,Santiniketan, India.

2. Lakshmi S Mohan, For the INO collaboration, “Hadron energy resolution as afunction of plate thickness and theta resolution of hadrons at the Iron CalorimeterDetector in India based Neutrino Observatory”, Proceedings of NUFACT 2013,IHEP, Beijing, China.
3. Gonzalo Mart´ınez-Lema, Lakshmi S. Mohan, Maddalena Antonello and IzabelaKochanek, “Hands on ICARUS: reconstruction of _μ charged-current events”,Proceedings of Gran Sasso Summer Institute 2014 Hands-On Experimental Un-derground Physics at LNGS, accepted to be published in Proceedings of Science.
4. Ahmed et al., The ICAL collaboration, “Physics Potential of the ICAL detectorat the India-based Neutrino Observatory (INO)”, arXiv:1505.07380 [physics.ins-det], 2015.1

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155. Name : **Narasimha Anaganti**
Enrolment No. : LIFE01201104002
Date of Award of degree : 26.12.16
Constituent Institute : Bhabha Atomic Research Centre,
Title : Characterization of selected radiation induced gene promoters in Deinococcus radiodurans R1

Abstract

Deinococcus radiodurans R1 survives exposure to extremely high doses of ionizing radiations, through distinct radiation responsive gene expression. However, the underlying gene regulatory mechanisms are not adequately understood. Comparative genomics has revealed presence of a 17 bp palindromic *cis*-regulatory element, called the Radiation Desiccation Response Motif (RDRM), in 24 radiation inducible genes. To understand their regulation, a third generation promoter probe shuttle vector pKG was constructed, using the green fluorescent protein (GFP) as a reporter. The vector exhibited undetectable GFP fluorescence in *Escherichia coli* or *Deinococcus radiodurans*. The utility of vector for *in situ*, visual and quantitative evaluation of promoters was validated for two known *D. radiodurans* promoters P_{groESL} and P_{ssb}. Assessment of 20 promoters cloned in the pKG vector showed that (a) conserved -10 and -35 like sequences were essential for promoter activity in *E. coli*, but were dispensable for gene expression in *D. radiodurans*. (b) RDRM-based promoters showed low basal GFP expression in *D. radiodurans*, but did not affect gene expression in *E. coli* (c) RDRM was necessary for radiation induction of all RDRM-based promoters (d) RDRM repressed the promoter activity when inserted into non-RDRM promoters (e) RDRM effected radiation-induced gene expression when placed in the proximity of core promoter but not if it was far upstream or downstream of the core promoter. DdrO repressed the activity of all RDRM containing promoters in *E. coli*. PprI, which cleaves DdrO protein *in vitro*, was essential for *in vivo* radiation induction of RDRM promoters in *D. radiodurans*. RDRM sequence mutants revealed that perhaps RDRM also serves an activator-like function for higher expression yields upon repressor clearance post-irradiation. The results extend the existing RDRM/DdrO/PprI based regulation model in *D. radiodurans*, to evolve both a negative as well as a positive role of RDRM in regulation of DDR regulon.

Publications

Journal

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conference/seminars

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2. Ananganti Narasimha, Bhakti Basu and Shree Kumar Apte, "Radiation and Desiccation Response Motif mediates radiation induced gene expression in *D. radiodurans",* in Life Science Symposium during 3rd-5th Feb 2015. (Received Best poster Award)
3. Anaganti Narasimha, Bhakti Basu and Shree Kumar Apte"Radiation responsive gene promoters in *Deinococcus radiodurans* are regulated by radiation and desiccation response motif (RDRM)", International Conference on Bacterial Expression-II held at NCBS Bengalore, India, during 1-5th Dec 2015, P.42.
4. Anaganti Narasimha, Bhakti Basu and Shree Kumar Apte "Radiation responsive promoters of *Deinococcus radiodurans*", International Conference on Radiation Research: Impact on Human Health and Environment (ICRR-HHE 2016), held at Anushaktinagar, Mumbai, India, during Feb 11-13th 2016.

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156. Name	:	**Mrityunjay Tyagi**
Enrolment No.	:	LIFE01201104003
Date of Award of degree	:	26.12.16
Constituent Institute	:	Bhabha Atomic Research Centre,
Title	:	Mechanistic Insight Into Malabaricone C Induced Cancer Cell Death.

Abstract

Background-Given that lung cancer is the second leading cause of cancer-related deaths with low survival rates, we explored the anticancer potential of malabaricone C (mal C), present in the methanolic extract of *Myristicamalabarica*(rampatri) a well-known spice of Indian cuisines for developing an efficient drug with minimum side effects and rationalize its action mechanistically.Methods- Cytotoxicity and induction of apoptosis was shown by MTT, Annexin V-FITC and Sub-G1. Mitochondria deficient cells, shRNA-mediated BCL2, p53 and ATM depleted cells and pharmacological inhibition of DNA-damage response proteins and MAPKs were employed to explore the signaling mechanism. Western blotting, immunoprecipitation and confocal microscopy were used to explore the pathway. Results- Mal C showed better killing of the cancer

cells than curcumin and etoposide. DNA damage generation in Mal C treated cells is paralleled with the induction of ATM- and ATR-mediated CHK1 phosphorylation. It was followed by p38-MAPKs and p53 dependent imbalance in BAX/BCL2 expression and cytochrome-c release. ATM silencing and ATR inhibition partially attenuated the mal C-induced p38-MAPK activation, CHK1 phosphorylation and apoptosis. Induction of DNA damage by mal C involved ROS generation. Thiol antioxidants enhances mal C induced apoptosis by: 1) Regenerating mal C, 2) Inhibiting transcription dependent function of proteins like NF- B and p53 and 3) S-glutathionylating p53 to induce its mitochondrial accumulation and cyt c release. Imperatively mal C and thiol antioxidant treatment reduced tumor burden in two different mice models. Conclusions-Mal C activates different cascade of events to cause mitochondria dependent cell death in lung carcinoma cells and thiol antioxidants enhances this process. The present findings with mice tumor models advocate mal C to be a potential anti-cancer agent for further evaluation.

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1. "DNA damage dependent activation of checkpoint kinase-1 and mitogen- activated protein kinase-p38 are required in malabaricone C-induced mitochondrial cell death", M. Tyagi, R. Bhattacharyya, A. K. Bauri, B. S. Patro and S. Chattopadhyay. BiochimicaBiophysicaActa (BBA) - General Subjects,2014, 840(3), 1014–1027.
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Conferences

1. International Conference on recent trends in therapeutic advancement of free radical science and 10th annual meeting of the SFRR-India -2011 (Chennai, TN) – Poster Presentation.
2. International Conference on recent trends in free radical and antioxidant research and 13th annual meeting of the SFRR-India-2014(Lonavala, MH) - Poster Presentation.

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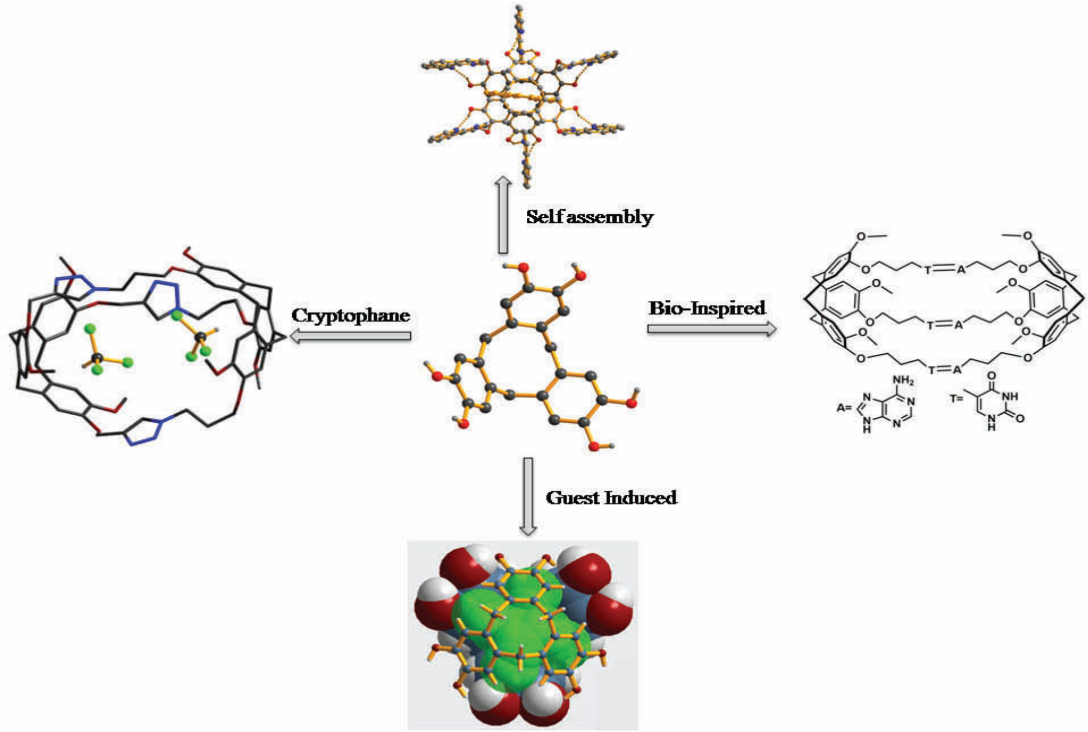
157. Name : **Pardhasaradhi Satha**
Enrolment No. : CHEM11201004003
Date of Award of degree : 04.01.17
Constituent Institute : National Institute of Science Education and Research,
Title : Cyclotriveratrylene Based Molecular Capsules : Synthesis, Characterization and Guest Entrapment.

Abstract

Cyclotriveratrylene(CTV) and its derivatives which are macromolecules readily available in the bowl shape were shown to form cryptophanes, which were connected by covalent bond and some metalated cages. CTV and its derivatives based molecular capsules with aid of non- covalent interactions viz. hydrogen bonding, guest inducing has not been explored thoroughly. Hence, the main objective of this thesis is to investigate CTV based non- covalently linked molecular capsules. This thesis consists five chapters, Chapter **1** discuss about the molecular capsules that were reported in the literature. Chapter **2** discuss about the synthesis of hydrogen bonded molecular capsules with Cyclotricatchylene (CTC), and their guest entrapment properties.[1,2] Chapter **3** discuss about the synthesis of Cyclotriguaiacylene (CTG) based bioinspired molecular capsule.3 Chapter**4** discuss about the guest induced molecular capsules based on Cyclotricatchylene (CTC).4 Chapter **5** discuss about the synthesis of a triazole bridged cryptophane by joining two Cyclotriguaiacylene(CTG)units.5



Publications

Journal

1. Pardhasaradhi Satha, Giriteja Illa, Chandra Shekhar Purohit, *Cryst. Growth Des.* 2013, *13*, 2636.
2. Pardhasaradhi Satha*,* Chandra Shekhar Purohit,. *Proc. Natl.Acad. Sci., India, Sec.A Phys.Sci.* 2014, *84(2),* 221.
3. Pardhasaradhi Satha, Giriteja Illa, Arindam Ghosh, Chandra Shekhar Purohit, *RSC Adv*., 2015, *5,* 74457.
4. Pardhasaradhi Satha, Giriteja Illa, Arindam Ghosh *,* Chandra Shekhar Purohit. *Chemistry Select* 2016, *1,* 1630

Communicated

1. First synthesis of a triazole bridged Cryptophane and guest entrapment studies Pardhasaradhi Satha, Giriteja Illa, Chandra Shekhar Purohit

158\. Name : **Woormileela Sinha**
Enrolment No. : CHEM11201004003
Date of Award of degree : 04.01.17
Constituent Institute : National Institute of Science Education and Research,
Title : Synthesis, Structures, Spectroscopic Characterization And Oxidation State Distributions In Metallocorroles.

Abstract

Corroles are tetrapyrrolic aromatic macrocycles resembling the naturally occurring biological pigments, porphyrins and corrins. Corroles have recently gained a lot of research interest for its interesting structural and spectroscopic properties. In this thesis, various scaffolds of corrole frameworks and their corresponding metalated derivatives have been explored on the basis of either biological or physical significances. Efforts are laid to comprehend the mechanistic aspects of their reactivity and also electronic, structural and spectroscopic changes on electron transfer in individual cases.In separate studies, oxidation state distributions in corrolato iron nitrosyl complexes, semi-insulating device fabrication with nanoaggregates of tin(IV) corroles, efficient and mild demetalation strategy of tin(IV) corroles have been investigated. Oxidation state distributions in corrolato iron nitrosyl complexes, studied here will be useful to comprehend their role in redox catalytic reactions. While the semi-insulating property of the tin(IV) corroles can be directly implemented for the construction of high-electron-mobility transistors (HEMT) in modern communication devices after adequate precise optimizations, the acid-free efficient demetalation strategy will be definitely useful in performing various organic transformations. Furthermore, oxidized forms of monomeric silver(III) and copper(III) complexes of corroles have been found to behave as near-IR absorbing dyes. Thus suitable design of such systems may lead to the discovery of newer varieties of chlorophyll-like light-harvesting units that may not solely depend on the photosynthetic special-pairs.With the simultaneous stabilization of unusual oxidation states of metals, e.g. Ag^{II} and Cu^{IV} forms on one-electron reduction of silver(III) corroles and one-electron oxidation of copper(III) corroles respectively can lead to interesting reactivity patterns, where metal-ligand cooperativity may be used for bond activation reactions and catalysis.

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2. *Sinha, W., Sommer, M. G., Deibel, N., Ehret, F., Bauer, M., Sarkar, B., Kar, S. Experimental and Theoretical Investigations for the Existence of Cu(II), Cu(III) and Cu(IV) in Copper-Corrolato Complexes. *Angewandte Chemie International Edition* 2015, DOI 10.1002/anie.201507330 and 10.1002/ange.201507330.
3. Garai, A.; Kumar, S.; Sinha, W.; Purohit, C. S.; Das, R.; Kar, S. A comparative study of optical nonlinearities of trans-A_2B-corroles in solution and in aggregated state. *RSC Advances* 2015,*5* (36), 28643-28651.
4. *Sinha, W.; Sommer, M. G.; Deibel, N.; Ehret, F.; Sarkar, B.; Kar, S. Silver Corrole Complexes: Unusual Oxidation States and Near-IR-Absorbing Dyes. *Chemistry-A European Journal* 2014,*20* (48), 15920-15932.

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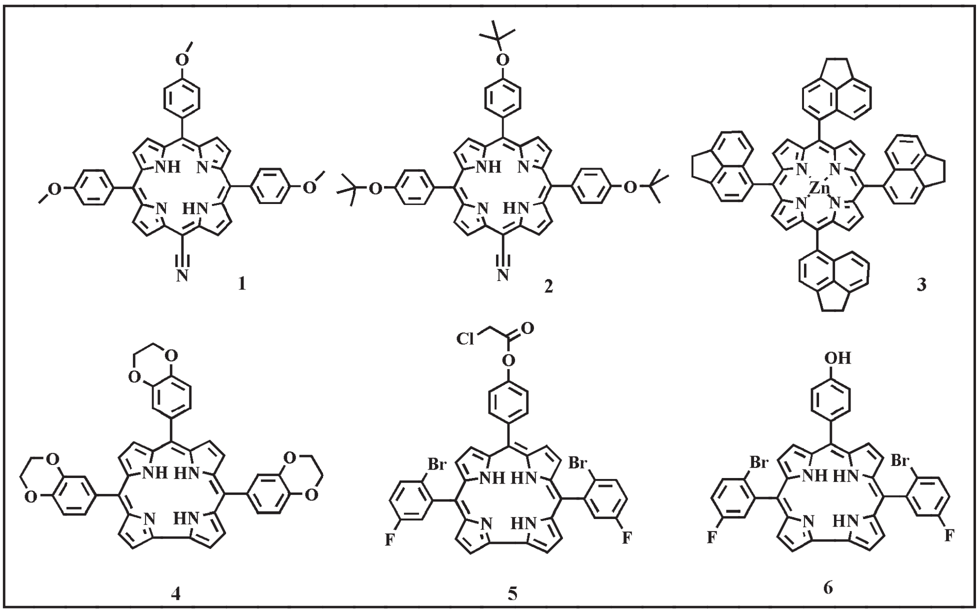
159. Name : **Antara Garai**
Enrolment No. : CHEM11201004004
Date of Award of degree : 04.01.17
Constituent Institute : National Institute of Science Education and Research,
Title : Synthesis of Functionalized Porphyrins and Corroles and Their Applications in Materials Science.

Abstract

Porphyrin is basically C20 macrocycle where four pyrrole rings are connected *via* methine bridges (=CH). These tetrapyrrolic systems have numerous applications including catalysis, photodynamic therapy, sensors, and NLO materials. First chapter deals with general introduction about porphyrin and one *meso* carbon contracted porphyrinoid, corrole. In the second chapter a novel two step one pot synthesis of cyanoporphyrin (**1, 2**) has been reported. This protocol does not require any porphyrin /metalloporphyrin based starting materials and additional reagents for cyanation as DDQ is performing dual role of cyanation as well as oxidative macrocyclization. Third chapter deals with fabrication of ZnP, **3**-fullerene based nano-architecture based MIS type diode and future application as charge storage devices. In forth chapter, NLO properties of a series of novel corrole systems (**4**, **5**, **6**) both in solution state and in aggregated state are discussed. Detailed investigation dictates that these corrole systems could be potential promising candidates in their aggregated state for devising optical switch in high-speed communication technology.



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160. Name : **M. Ramakrishnan**
Enrolment No. : PHYS02201004020
Date of Award of degree : 09.01.17
Constituent Institute : Indira Gandhi Centre for Atomic Research,
Title : Classical And Dynamic Approaches To Probabilistic Safety Analysis Of Fast Reactors.

Abstract

Reactor safety analysis is vital to understand and ensure that the risk to public is acceptably low. Probabilistic safety Analysis plays an important role in the safety analysis of nuclear power plants. Traditional PSA approaches like fault tree and event tree are applied to typical Fast Breeder Reactor (FBR) which is under construction. The level-1 internal events PSA is carried out for this reactor. This study identifies the dominant contributors to core damage frequency. Insights on the design of this plant and the role of common cause failures in Probabilistic Safety Analysis (PSA) are understood from this study. The importance of external events in the safety assessment of nuclear power plants was demonstrated by the Fukushima accidents. The level-1 external events PSA is carried out for the first time for a pool type FBR. Seismic events and flood are the two external events considered. Site specific seismic hazard analysis is carried out. This study validates the design basis ground motion parameters obtained from deterministic hazard analysis. Plant specific data is used for fragility to the possible extent. A method to estimate median acceleration capacity from seismic qualification experiments was identified. The core damage frequency due to seismic events was calculated. The plant under consideration is located on the east coast of India. Flooding events is one of the external events to be considered. Of the different possible flooding events, Tsunami is the governing event for this plant. Tsunami hazard analysis by including the local bathymetry was carried out. The inclusion of bathymetry increases the tsunami wave run up height predictions. The safety systems and equipments of this plant are located at ~9.6m above Mean Sea Level. Tsunami waves with run up height equal to or above this value has the potential to affect the safety systems of the plant. The probability of occurrence of such tsunami waves is small as estimated from tsunami hazard analysis. The core damage frequency due to external flood is expected to be small due to the above mentioned reasons. Two different accident sequence models for flood PSA are compared.There are two elements in a safety system analysis. They are the physical process involved (e-g: neutronic, thermal hydraulic etc) and the hardware / human components involved in the safety system function. Traditional PSA approaches like fault tree and event tree take input from process analysis for deriving the success / failure criteria, mission time etc. With the evolution of innovative designs of reactor safety systems, improved methods to quantify various reliability measures are needed. Also the time dependent interaction between the process and system hardware / human is to be considered. Dynamic PSA is a tool to meet the above challenges. Dynamic PSA is an integrated model in which both process and system hardware evolves with time. The time dependent interactions between process and hardware are modelled. Dynamic PSA quantifies both the uncertainties in process and stochastic changes in system hardware. Monte Carlo simulation for system hardware is one of the requirements for dynamic PSA. Different Monte Carlo simulation schemes are applied to the shutdown system of a FBR and the results are compared. An efficient Monte Carlo simulation scheme for system hardware is identified. This simulation scheme is combined with a process model in a simple example. This example study is used to validate the simulation algorithm. The passive decay heat removal system of a FBR is modelled by combining the evolution of hot pool temperature with the Monte Carlo simulation of system hardware. The results from this study are compared with functional reliability analysis and functional reliability analysis combined with fault tree for system hardware modelling. The results from these three methods are significantly different when the process uncertainty contribution to total failure probability is not dominant and results converge when the process uncertainty contribution to total failure probability is dominant. Dynamic PSA approach reduces the conservatism in failure probability estimation in functional reliability analysis combined with fault tree approach. An attempt to explain the applicability of different methods based on process uncertainty is made.

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2. M.Ramakrishnan, A. John Arul, V.Bhuvana, P.PuthiyaVinayagam and P. Chellapandi,"Accident Sequence Modeling Methodology for External Flood Probabilistic SafetyAnalysis of Prototype Fast Breeder Reactor", Applied Mechanics and Materials, Vols.592-594 (2014), pp 2460-2464.
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2. M.Ramakrishnan, A. John Arul, V.Bhuvana, P.PuthiyaVinayagam and P. Chellapandi,"Accident Sequence Modeling Methodology for External Flood Probabilistic Safety Analysisof Prototype Fast Breeder Reactor"- Presented in International Mechanical EngineeringCongress (IMEC-2014) held at NIT, Trichy, June 13-15, 2014.
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161. Name : **Hitesh V. Rahangdale**
Enrolment No. : PHYS05201004011
Date of Award of degree : 09.01.17
Constituent Institute : Saha Institute of Nuclear Physics,
Title : Electron Impact Ionization Study of High Z elements

Abstract

This thesis is based on experimental and simulation work broadly in the area of Atomic Physics. Specifically, we have measured electron impact ionization cross-sections by performing electron-atom collision experiments with solid targets and detecting X-rays. By observing X-rays from electron-atom collision experiments with solid films various phenomenon can be studied such as bremsstrahlung process, alignment studies of various atomic subshells, or cross section measurement of particular transitions. In this regard electron-atom collisions leading to the ionization of K shell and related transitions is extensively studied and is very well explained by theories, but fewer studies exist for the L (2*s*,2*p* etc.) and M (3*s*,3*p* etc.) shell ionization. In this thesis, we have taken this study further and studied electron impact L-shell ionization in high Z elements.The experimental part of the thesis involves instrumentation to develop Energy dispersive X-ray spectrometer for studying the electron impact ionization process. In this setup, electrons of energies 1–50 keV are bombarded on the thick or thin film targets and the emitted X-rays are detected with solid state detectors (Si-PIN diode and SDD). A separate setup for alpha energy loss spectroscopy was also developed to measure the thickness of the thin films needed for cross section measurement. Using the energy dispersive spectrometer we studied five high Z elements *viz.,* Au, Pb, Bi, U and Th, and obtained absolute X-ray production cross sections for L_α, L_β and L_γ, transitions and sub-shell resolved absolute ionization cross sections for L_1, L_2 and L_3 sub-shells.To eliminate the effect of bulk properties of thin films on the obtained cross sections, Monte Carlo simulation of electron transport in the thin films using GEANT4 and PENELOPE packages is performed. In GEANT4, the simulation is done using the low energy physics list *viz.* Livermore physics list and Penelope physics list. Using simulations, important quantities such as energy loss of projectiles inside target films and the number of collision per projectile are obtained and it was verified that no multiple collision occurs, for the used target in the experiment. Also, Bremsstrahlung spectra due to electron impact on thick Carbon and Aluminum films were generated from simulation, using which the efficiency of the Silicon Drift X-Ray Detector was determined.The experimentally obtained ionization cross sections are compared with theories such as Distorted Wave Born Approximation. On comparison it is found that although theoretical estimates are in agreement for L_3 subshell cross sections data, they are higher than our experimental results for L_1 and L_2 subshells. After obtaining the experimental ionization cross sections from different methods we have found that the discrepancy between the experiment and theory can be attributed to the atomic relaxation parameters (such as radiative Yields).

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1. "Determinationof subshell-resolved L-shell-ionization crosssectionsof goldinducedby15-40keVelectrons"Rahangdaleet. al, Phys.Rev.A 89,052708 (2014).
2. "Spectroscopicinvestigations of L-shellionizationin heavy elementsby electronimpact."Rahangdaleet. al,J.Quant.Spectrosc. Radiat.Transfer 174, 79-87(2016).

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162. Name : **Maitreyee Mukherjee**
Enrolment No. : PHYS04201004004
Date of Award of degree : 09.01.17
Constituent Institute : Variable Energy Cyclotron Centre
Title : Event-By-Event Multiplicity Fluctuations In High Energy Heavy Ion Collisions At The Lhc Energies In The Alice Experiment.

Abstract

Quark-Gluon-Plasma (QGP) is a state of matter, described by Quantum Chromo Dynamics (QCD), which may exist in extremely high temperature and energy-density. By colliding nuclei at ultra-relativistic energies, it is possible to create such an extreme environment, where this QGP-state of matter may exist. A Large Ion Collider Experiment (ALICE) at the Large Hadron Collider (LHC) of CERN is designed to study the properties of the strongly interacting matter. One of the basic advantages of the heavy-ion collisions at relativistic energies is the production of large number of particles in each event, which facilitates the event-by-event study of several observables. A non-monotonic behaviour of event-by-event multiplicity fluctuations may signal the onset of deconfinement, and can be used to probe the critical point in the QCD phase diagram. Multiplicity fluctuations are characterized by the scaled variances of the multiplicity distributions, defined as, $\omega_{ch}=\sigma^2/\mu$, where, σ^2 and μ are the variance and mean of the multiplicity distribution. Additionally, the ALICE experiment is able to access a novel regime where initial state effects can be studied very well with the help of the multiplicity fluctuation studies. In this thesis work, ALICE data analysis on the event-by-event multiplicity fluctuations is presented for charged particle multiplicity distributions produced in Pb-Pb collisions at $\sqrt{s_{NN}}$= 2.76 TeV and for p-Pb collisions at $\sqrt{s_{NN}}$= 5.02 TeV. For the work, detectors used are - Inner Tracking System (ITS) for vertex-selection and tracking, Time Projection Chamber (TPC) for tracking and V0 for centrality selection. Extensive studies have been performed for centrality selection, track selection, centrality bin width correction for non-uniformity in charged particle multiplicity distribution, correction of the results for the detector inefficiency (including the phase-space dependence of the efficiency factor), correction for contamination, error estimation for limited statistics and error estimation for the systematics arising from the experiment. A universal scaling in the multiplicity fluctuation observable has been presented. Multiplicity fluctuations are related to the isothermal compressibility (k_T) of the system produced in the high energy collisions. An estimation for the values of k_T has been done for Pb-Pb collisions at $\sqrt{s_{NN}}$= 2.76 TeV. Additionally, multiplicity distributions of produced particles and their event-by-event fluctuations are presented in the thesis using the AMPT model in the default and string melting modes for a large range of energies. In addition to being sensitive to the QCD phase transition, these fluctuations provide baselines for other event-by-event measurements.

Publications

Journal

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2. Centrality determination of Pb-Pb collisions at $\sqrt{s_{NN}}$ = 2.76 TeV with ALICE. Maitreyee Mukherjee (for the ALICE Collaboration), Phys.Rev. C88 (2013) 4, 044909. arXiv : 1301.4361 [nucl-ex].

Communicated :

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2. Charged Particle Multiplicity Fluctuations in Pb–Pb collisions at $\sqrt{s_{NN}}$=2.76 TeV in ALICE. Maitreyee Mukherjee (for the ALICE Collaboration), under Collaboration review.

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163. Name : **Sourav Pramanik**
Enrolment No. : PHYS05201104004
Date of Award of degree : 10.01.17
Constituent Institute : Saha Institute of Nuclear Physics,
Title : Nonlinear Particle Dynamics Of Plasma Diodes In Presence Of External Magnetic Field.

Abstract

An elaborate and comprehensive analysis has been made in this doctoral work to present a vivid picture of the steady state properties of the plasma diodes in the presence of the transverse magnetic field. To be more specific, the theoretical investigations presented in this doctoral work, is mainly focussed on the impact of the transverse magnetic field on the space charge limited flow, the maximum allowable current at steady state as well as on the aperiodic instabilities found in plasma diodes. For this purpose, we have used a planar model and derived the steady state solutions employing the simple fluid-equations (the continuity and momentum equation) along with the Poisson's equation for the electric field. The analysis is presented with the help of both Eulerian and Lagrangian descriptions. It is observed that the value of the maximum steady state current (space charge limited current) decreases when the magnitude of the external magnetic field is increased. All the stationary states are visualized through the "emitter electric field vs diode gap" parametric diagram. The steady state solutions can be distinguished into three categories which are represented by three distinct branches of the "emitter electric field vs diode gap"-curves. These branches are named as, Normal C branch, C-overlap branch and B-branch (or virtual cathode branch). The width of the C-overlap branch decreases with the magnetic field and at a particular strength of the applied magnetic field, C-overlap branch disappears. With the increasing strength of the external magnetic field, "emitter electric field vs diode gap"-curve gets displaced. As a result, a diode which was initially at a state with high current density (corresponding to Normal C branch) in absence of magnetic field, now shifts to another state with negligible current (which belongs to B-branch) as soon as a magnetic field of finite strength is applied along the transverse direction. As an important application of our results, an idea to develop a fast electronic switches is suggested, based on the state-transition phenomena observed in plasma diodes. For generalized

Pierce diodes, a new family of solutions is observed and it is found to be very sensitive to the magnetic field. The results of our works are believed to be applicable to the systems like thermionic energy converters, microwave emitters, low pressure discharge and processing devices, xerographic technologies, Q-machines etc where space charge limited current flow plays a major role.

Publications

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2. *Stability analysis of steady state solutions of Bursian diode in presence of transverse magnetic field*.S. Pramanik, V. I. Kuznetsov and N. Chakrabarti, *Physics of Plasmas* 22,082103 (2015).
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7. *Wave breaking of nonlinear electron oscillations in a warm magnetized plasma*.S. Pramanik, C. Maity and N. Chakrabarti, *Physics of Plasmas* 21, 022308 (2014).
8. *Phase-mixing of ion plasma modes in pair-ion plasmas*.S. Pramanik, C. Maity and N. Chakrabarti, *Physics of Plasmas* 22, 052303 (2015).
9. *The phase mixing of an upper hybrid wave in a magnetized pair-ion plasma*.S. Pramanik, C. Maity and N. Chakrabarti *Physica Scripta* 91, 065602(2016).

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164. Name : **Prasanta Char**
Enrolment No. : PHYS05201104001
Date of Award of degree : 10.01.17
Constituent Institute : Saha Institute of Nuclear Physics,
Title : Some Studies On Core-Collapse Supernovae And Neutron

Abstract

This thesis mainly focuses around some studies of the core-collapse supernovae (CCSN) to neutron stars (NS). In this work, I have tried to write a realistic equation of state (EoS) for dense matter with strange components and implement it to CCSN simulations. I have also studied the role of nuclear physics of the crust in the oscillation modes of neutron stars. Main motivation of this work is the recent measurements of masses of highly massive pulsars which have tremendous implications for constraining the NS EoS. Pauli exclusion principle dictates the appearance of strange hadrons in the high density baryonic matter resulting a softening of the EoS lowering the maximum mass of the star. The possibility whether in spite of softening of EoS, one can still manage to construct an EoS with strange matter and achieve a maximum mass $2M_{solar}$ within the observable limit is investigated. For this a density dependent relativistic field theoretical framework with hyperons, anti-kaon condensates is used. For hyperon-hyperon and kaon-baryon interaction, Φ-meson is used in addition to σ, ω and ρ mesons of usual extended RMF model. In this framework, I studied the EoS and the compositions of NS matter in β-equilibrium. It was observed that the appearance of strange baryons softened the EoS. However, in all the cases it is found that the maximum mass is always within the constraint of observational limits. Therefore, it is concluded that exotic EoS can not be ruled out by the observation of $2M_{solar}$ neutron star. The success of the density dependent hadron field theory model has led to its use in CCSN simulations. Recently, Λ hyperons have been added to this supernova EoS . A thorough comparative study is conducted between this new EoS (BHBΦΛ) and the widely used supernova EoS (HShenΛ). Both of these EoSs are applied into a one-dimensional spherically symmetric general relativistic (GR) code GR1D to study the dynamical collapse of a non-rotating massive star into a black hole. I have studied radial profiles of density, temperature and mass-fractions of the protoneutron star (PNS) at different instants of time, in great detail. The temporal evolution of density, temperature, mass-fractions, neutrino luminosity, shock radius etc. of the PNS have also been examined to carefully distinguish the effects of Λ hyperon on metastability of the PNS, the onset of BH formation etc. Normally, when the core region reaches density above twice the nuclear saturation density, the onset of Λ hyperons are energetically favored. As hyperons soften the EoS, black holes form much earlier than the nucleon-only case. I also studied with a $20M_{solar}$ progenitor model similar to the progenitor star of SN1987A and induced an explosion with artificial neutrino heating and studied the long duration time evolution of the remnant. It is found that the shock radius kept expanding continually and the PNS remaining stable after considerable amount of time. The other part of the thesis is the study of the oscillation of highly magnetized neutron stars. It involves the study of the effect of a strongly magnetized crust using the SLy4, SkM and Sk272 nucleon-nucleon interactions and the shear modulus calculated from these models on the frequencies of torsional shear modes as well as the global Alfvén modes. It is observed that the increase in shear modulus, because of the Landau quantization of the electrons, does not affect the frequencies of fundamental torsional shear modes. But, the frequencies of the first overtones are markedly different in the strong field case from field-free case. The effect of crust is found to disappear above a critical magnetic field ($B > 4 \times 10^{15}$ G) and both the torsional shear and Alfv´en oscillations become global magnetic oscillations. Finally, the calculated frequencies using different stellar models, magnetic fields and magnetized crusts are compared with observed frequencies for SGR 1806-20, SGR 1900+14.

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2. A Comparative Study of Hyperon Equations of State in Supernova Simulations.Prasanta Char, Sarmistha Banik, Debades Bandyopadhyay;Astrophysical Journal 809 (2015) 116 [arXiv:1508.01854]
3. Role of Nuclear Physics in Oscillations of Magnetars .Rana Nandi , Prasanta Char , Debarati Chatterjee, Debades Bandyopadhyay;Physical Review C 94 (2016) 025801 [arXiv:1608.01241]

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1. Core Collapse Supernova Simulation using Λ-hyperon EoS with Density Dependent CouplingsSarmistha Banik, Prasanta Char, Proceedings of 20th International Conferenceon Particles and Nuclei (PANIC 14), 24-29 Aug, Hamburg, Germany, p.391-394(doi:10.3204/DESY-PROC-2014-04/115).
2. Comparison of Hyperonic Equations of State for Core Collapse Supernovae SimulationsPrasanta Char, Sarmistha Banik,Astronomical Society of India Conference Series, 2015, Vol. 12, pp 115-116

165. Name : **Sanjima Pal**
Enrolment No. : LIFE11201004004
Date of Award of degree : 10.01.17
Constituent Institute : National Institute of Science Education and Research,
Title : Biological studies on different cellular responses to bioactive compounds of natural and synthetic origin.

Abstract

Biologically active compounds of natural or synthetic origin have been in use for both disease prevention and cure since time immemorial. The increasing global burden of diseases necessitated scientists to discover and develop new interventions resulting in a commendable progress in science and medicine. My doctoral thesis was focused on establishing undefined bioactivities of a hormetic phytochemical, sulforaphane and characterizing few benzo[α]phenoxazines for anticancer activity and their mode of cell death.Sulforaphane (SFN) is a hormetic agent well-studied for its anticancer activity, but nevertheless is also an anti-inflammatory agent whose direct effect on auto-reactive monocytes/macrophages has not been critically assessed. The first part of the thesis elaborates a non-cytotoxic (especially non-apoptotic), MAPK (activity) dependent function and phenotype switching (M1/M2) ability of SFN during and after monocytes to macrophage differentiation (PMA induced) of human monocytic cell line, THP1. Here, the ability of SFN to suppress in vitro soluble collagen-induced autoimmune inflammatory condition was demonstrated. Further, the ability of SFN to change the phenotype and function of spontaneously differentiating primary human monocytes/macrophages (peripheral blood derived) in favor of a specific anti-inflammatory M2 type that can suppress soluble collagen induced autoimmune condition was investigated. From the studies, it was observed that SFN can suppress in vitro inflammation (soluble collagen induced) by targeting the altered endogenous FasL maturation (absence of 26 KDa cleaved product) in autoreactive M1 cells (THP1 derived) during and after their polarized differentiation .Benzo[α]phenoxazines (BPZ) class of compounds are known fluorescent dyes where few studies report their inhibitory role in chemorefractory malignancy. In the thesis, three novel synthetic derivatives of BPZs, 1B (10-chloro-benzo[α]phenoxazine-5-one), 2B (10-methyl-benzo [α]phenoxazine-5-one) and 3B (benzo[α]phenoxazine-5-one) were studied in vitro for cell-specific (colon and pancreatic) anticancer activities. Efforts were specifically made to comprehend their activity in different assays (cell cycle arrest, followed by cell death via apoptosis or autophagy) following uptake into the cells. Cumulatively, the thesis highlights and sheds light on new immune-regulatory role and anticancer activity of SFN and BPZs respectively.

Publications

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166. Name : **Juby K. Ajish**
Enrolment No. : CHEM01201104016
Date of Award of degree : 13.01.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Synthesis And Study Of Carbohydrate Based Hydrogels And Self Assembled Glycoacrylamides For Biomedical Applications.

Abstract

Polymers and macromolecules in general have become a major part of our day to day lives that it has become a necessity. As per the requirement or application they are used in various forms, like hydrogels, nanoparticles, thin films, spherical beads so on and so forth. Using radiation technology it is now possible to synthesize nanoparticles incorporated hydrogel matrices *in situ*. A simple one-pot method for in-situ synthesis of silver nanoparticles (AgNPs), within polyvinyl alcohol-gum acacia (PVA–GA) hydrogel matrix, by γ-radiation induced cross-linking was used. The synthesized gels were tested for thermal stability, equilibrium swelling, AgNPs release kinetics, size of AgNPs leached out and its dependence on the antibacterial activity against E.*coli* bacteria. Major objective of this study was to determine how the size and rate of leaching out of AgNPs affect the antibacterial activity. It was observed that higher the crosslinking density, smaller is the size of AgNPs and better is the antibacterial activity, even though the rate of leaching is slow. A radiation dose of 25.34 kGy was calculated to be the gel point which is close to the sterilization dose for biomedical applications. D-glucose based bisacrylamide substituted at C-3 and C-6 carbon of sugar (Glc-bis) and monoacrylamide substituted at C-6 position (Glc-acryl) was synthesized and their gelation was studied using radiation polymerization. Glycopolymeric hydrogels were synthesized using these glucose based derivates by radiation induced crosslinking. The molecular structure, water content, viscoelasticity, thermal stability, cytotoxicity and lectin recognition of the synthesized hydrogels (Glc-gel) were studied using the techniques, like FT-IR spectroscopy, Oscillatory rheology, Thermogravimetric-Differential Scanning Calorimetric (TG-DSC) analysis, MTT assay and UV-vis spectroscopy. The ability of sugar pendants in glycopolymers to mimic that on the cell surface makes them a unique class of materials for targeted drug delivery applications. *N*-succinyl chitosan (NSC) based hydrogel beads, stabilized with glycopolymeric network (NSC/Glc-gel), for application in delivery of anticancer drug, doxorubicin (DOX). The Glc-gel, made

from bisacrylamide (Glc-bis) and monoacrylamide (Glc-acryl) monomers derived from D-glucose, would provide the required stability for the NSC beads against dissolution upon drug loading, and could control the drug release. The beads exhibited sustained release of DOX over a period of more than 15 days in an acidic environment, mimicking the microenvironment of tumor cells. While the rate of DOX release at physiological pH was found to be much slower. Release exponent 'n' derived from Korsmeyer-Peppas model implied that the NSC88/Glc-gel beads with 88% succinylation of chitosan followed fickian diffusion controlled release mechanism, whereas the NSC75/Glc-gel beads with 75% succinylation of chitosan followed zero order release profile. The synthesized beads also showed specificity to lectin Concanavalin A. This stabilized polysaccharide based glycopolymeric gel bead could be a suitable base for pharmaceutical applications. The glucose based C-6 acrylamide (Glc- acryl) and C-3, C-6 bisacrylamide (Glc-bis) exhibit pH dependent self assembly with fluorescent emission. The building blocks contain hydrophobic acrylamide units which act as the fluorescent probe by virtue of its stacking through weak π-π interaction and the hydrophilic glucose units serve as the lectin binding moiety. Significant fluorescence enhancement upon interaction with Con A arising due to enhanced Aggregation Induced Emission (AIE) effect was studied. The biocompatibility and cell uptake behaviours of Glc-acryl and Glc-bis were also studied using human intestinal cell lines (INT407), as it contain receptors which can specifically identify D-glucose moieties

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3. Silver nanoparticle loaded PVA/gum acacia hydrogel: Synthesis, characterization and antibacterial study.
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4. Fluorescence turn-on sensing of lectins and cell imaging based on aggregation-induced emission of glycoacrylamides.
   Juby K. Ajish, K. S. Ajish Kumar, Mahesh Subramanian, S. Chattopadhyay, Manmohan Kumar, *RSC Advances,* 2016 (Communicated).

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167. Name	:	**Minal Yesuraja Nadar**
Enrolment No.	:	PHYS01201304013
Date of Award of degree	:	13.01.17
Constituent Institute	:	Bhabha Atomic Research Centre,
Title	:	Evaluation Of Parameters Influencing The In-Vivo Radioactivity Measurements And Uncertainties Due To Internal - Contamination Of Actinides.

Abstract

Assessment of internal contamination of radionuclides in radiation workers forms anintegral part of the radiation protection programme in nuclear facility. When contaminants are actinides, which are low energy photon emitters, detection becomes difficult due to attenuation of low energy, low yield photons in overlying tissues. For accurate estimation of lung/ GI tract/ wound activities by external detectors, it is important to evaluate the uncertainties introduced by various parameters. With this aim, uncertainties in lung activity measurements are evaluated using experimental and Monte Carlo methods. The parameters studied, mainly for lung activity estimation are: muscle equivalent chest wall thickness, positional errors, uncontaminated adult male background variation, variation of ^{239}Pu and ^{241}Am activity ratio in the lungs, non-uniform distribution of activity in lungs, counting statistics and contribution of source in other organs such as liver, skeleton and lymph nodes in lung measurements. Uncertainties are evaluated for all the parameters in the form of scattering factors (SFs) for Phoswich and HPGe array. Combined SF obtained from the SFs of each parameter is found to be ~ 1.35 and 1.47 for Phoswich and HPGe array respectively at and above 60 keV for lung activity assessment.Studies are also carried out to evaluate the uncertainties due to important parameters in the estimation of GI tractandwound activity due to internal contamination of actinides. Parameters studied are variation of GI tract activity with respect to time of ingestion intake and depth of embedded activity and tissue equivalent material used for calibration in case of wound intakes. It is found that to estimate ingested activity by direct measurements, counting efficiencies based on true activity distribution as per the solution of Human Alimentary Tract model should be used; otherwise, an error of ~ -16 to -75 % will occur in the assessed ingested activity. A methodology is developed to estimate the depth and wound activity embedded in wound for pure ^{241}Am and mixed ^{239}Pu, ^{241}Am compounds. The thesis also addresses intake estimation using enhanced urinary excretion data by mathematical modeling of modifiedbiokinetic models, when DTPA is given intravenously for multiple times. A methodology is developed for intake evaluation using 20 days urinary excretion data when DTPA is given intravenously single or multiple times.The study has key findings and will lead to accurate and realistic estimation of lung, GI tract and wound activities as well as intake evaluation for intravenous administration of DTPA.

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6. In-vivo Measurement of Pu/Am activity in liver using phoswich detector,Lokpati Mishra, I.S.Singh, Minal Y. Nadar, and D.D.Rao, Proc. IARPNC-2014, March 19-21, 2014Mumbai, 120.
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168. Name : **Dibyendu Bandyopadhyay**
Enrolment No. : CHEM01201004007
Date of Award of degree : 06.02.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Structure and Dynamics of Water in Bulk and at Molecular and Nanoscopic Interfaces: A Molecular Dynamics Simulation Study.

Abstract

Publications

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1. Properties of Heavy Water in the Temperature Range T = 223 K to 373 K fromMolecular Dynamics Simulation Using the Simple Point Charge/Heavy Water (SPC/HW)Model.Bandyopadhyay, D.; Mohan, S.; Ghosh, S. K.; Choudhury, N. *J. Chem. Eng. Data*, 2012, *57*,1751−1758.
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3. Comparison of Orders, Structures and Anomalies of water: A Molecular DynamicsSimulation study.Bandyopadhyay, D.; Mohan, S.; Ghosh, S. K.; Choudhury, N. *AIP Conf. Proc.* doi.10.1063/1.4791175, 2013, 1512. 590-591.
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169. Name : **Debabrata Chattaraj**
Enrolment No. : CHEM01201104022
Date of Award of degree : 06.02.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Studies On Hydrogenation Behavior Of Zirconium And Uranium Based Alloys

Abstract

One of the most important requirements for fusion reactor is tritium isotope (T or 3H)which is going to be used along with deuterium (D or 2H). Tritium is producedthrough nuclear reactions in a lithium-bearing blanket. Thereafter, it is extracted, purified, and stored. But, this radioactive isotope is a beta emitter. Hence, for the safe nstorage of this radioactive isotope, a suitable material is required to prevent the release of tritium into the environment. The solid state storage of hydrogen isotopes is quite reliable, safe and advantageous compared to gaseous or liquid form of storage. Metal hydrides are unique choice as solid state storage material for tritium. Development and delivery of such systems for tritium are of urgent requirement in the International\ Thermonuclear Experimental Reactor (ITER) program. Conventionally, uranium is used as “getter bed” for tritium as it has high absorption capacity at room temperature, low equilibrium pressure (<1 bar at 550–680 K) which prevents the accidental release of tritium into atmosphere, fast kinetics of hydrogen absorption–desorption and large thermal cyclic life. However, uranium hydride is pyrophoric in nature and also uranium is a nuclear material. So investigation for finding out an alternate material for tritium storage is in progress. The property of uranium can be improved by alloying it with titanium which can impart durability against powdering on hydrogenation and mcan reduce the pyrophoricity to a certain extent. Zirconium is also good for hydrogenisotope storage, but the main drawback is that the dissociation of hydrogen from zirconium hydride (ZrH2) requires moderately high temperature. Presently, the intermetallic ZrCo has been found to be suitable for the safe storage of tritium. ZrCo intermetallic has good hydriding/dehydriding property which can serve as a substitution of uranium. Also it is not pyrophoric and easy to handle as it is not a xv nuclear material. However, the major drawback of ZrCo is that its absorption–desorption cycle become poor on prolonged thermal cycling which is due to the disproportionation of its hydride (ZrCoHx (x ≤ 3) into the stable hydride phase ZrH2 and the hydrogen non-absorbing phase ZrCo2. To overcome the drawbacks of this system a fundamental study of physicochemical properties of ZrCo and its hydrides are required. Regarding hydrogen isotope storage, the isotope effect of ZrCoX3 (X = H, D and T) compounds are also of prime importance and required to be explored. In literature, researchers have reported the physico-chemical properties of tritium storage alloys and their hydrides both experimentally and theoretically to a certain extent. The properties of radioactive tritides are still lacking in the literature. A comprehensive study of fundamentalphysico-chemical properties like structural, electronic, elastic, vibrational and thermodynamic properties of those alloys and their hydrides is the main scope of this thesis. Apart from these, a large variety of thermo-chemical and thermo-physical properties of metals, alloys and their hydrides can be calculated theoretically whichcan support the experimental findings. Another important aspect of hydrogen storage materials is diffusion of hydrogen through the bulk metal or alloy. The

diffusion path, mechanism, activation barrier and temperature dependent diffusion coefficient are of prime importance for the gas-solid interacting systems. The investigation of diffusion phenomena may help to overcome the drawbacks related to hydrogen absorptiondesorption process. The hydrogenation behavior changes with the change in dimension of the hydrogen storage materials. Thus, it is also interesting to study how hydrogen interacts with the metals and alloys in the different dimensions like bulk, surface and nanoclusters. Xvi This thesis is divided into seven chapters as outlined below. Chapter 1: Introduction; Chapter 2: Theoretical Approach; Chapter 3: Experimental methods; 4: Theoretical and experimental study of U2Ti alloy 5: Theoretical and experimental study of Zr-based compounds 6: First principles study of hydrogeninteraction with ZrCo surface and clusters 7: Conclusions

Publications

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3. High temperature enthalpy increments and thermodynamic functions of U2Ti, D. Chattaraj, Ram Avtar Jat, S.C. Parida, Renu Agarwal, Smruti Dash*,Journal of Thermal Analysis and Calorimetry, 2013, 112, 141-145.
4. First principles study of ZrX2 (X=H, D, T) compounds,D. Chattaraj*, S.C. Parida, Smruti Dash, C. Majumder, International Journal of Hydrogen Energy, 2014, 39, 9681-9689.
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7. Atomic, Electronic and Magnetic Properties of Bimetallic ZrCo clusters: A FirstprinciplesStudy, D. Chattaraj, Saswata Bhattacharya, Smruti Dash, C. Majumder Journal of Applied Physics, 2016, 120, 094301 (p. 1-6)
8. Adsorption, dissociation and diffusion of hydrogen on the ZrCo surface and subsurface: A comprehensive study using first principles approach D. Chattaraj*, Nandha Kumar, Prasenjit Ghosh, C. Majumder, Smruti Dash(Submitted to Physical Review B, Manuscript reference number: BY12596)

170. Name : **Rushikesh Sudam Patil**
Enrolment No. : LIFE09201004010
Date of Award of degree : 07.02.17
Constituent Institute : Tata Memorial Centre
Title : Understanding pathogenesis of gallbladder cancer: Role of Th17 and Regulatory T cells.

Abstract

Gallbladder Cancer (GBC) is a relatively uncommon but lethal biliary tract related cancer with 5 year survival less than 5%.Complete surgical resection is the only curative option available, but more than 90% GBC patients are with un-resectable disease. Despite improved results of chemotherapy and surgery, the long term outcome remains disappointing. 70-80% patients are associated with chronic inflammatory condition of cholelithiasis. The present prospective study aimed at investigating the role of inflammatory immune infiltrates contributing to GBC. Immunophenotyping in GBC patients revealed thatthe cells contributing to adaptive immunity (CD3$^+$, CD4$^+$, CD8$^+$ T cells) were decreased in peripheral blood of GBC patients compared to healthy individuals (HI). Downregulated expression of CD3-ξ chain in T cells,low lymphocyte proliferative response and decreased secretion of effector cytokines upon stimulation with anti-CD3 mAb and mitogen suggests that the immune response in GBC patients is dysfunctional. Investigation of inflammatory immune cells revealed that the levels of IL17 producing subtype of γδ-TCR$^+$(Tγδ17), CD4$^+$ (Th17) and CD8$^+$ (Tc17) T cells were increased in peripheral blood (PBL) and tumor infiltrating lymphocytes (TIL) of GBC patients compared to HI. The data demonstrated that Tγδ17 cells specifically secrete IL17 and elicit production of VEGF and other angiogenesis related factors in gallbladder tumor cells.Tγδ17 also induced vascularization of chorioallantoic membrane through IL17. Addition of recombinant IL17 to gallbladder tumor cells (OCUG1 cell line) induced proliferation, migration, matrigelinvasion and VEGF productionin concentration dependent manner. For the first time it was shown that Tγδ17 cells migrate towards gallbladder tumor using CXCR3/CXCL9 chemokine axis. The cytokines required for differentiation and/or stabilization of Tγδ17 cells (IL6, IL23, IL1β) were elevated in the sera as well as in the tumor environment of GBC patients. Analysis of CD4$^+$CD25$^+$CD127$^{low/-}$regulatory T cells revealed that the levels of Tregs were decreased in PBL but their suppressive potential was not compromised. Study of dynamics of these cells revealed that in TILs, the ratios of Th17/Treg, Tγδ17/Treg and Tc17/Treg increased but CD8$^+$IFNγ$^+$ and γδ$^+$IFNγ$^+$ cells were decreased. Moreover, Tγδ17, Th17 and Tc17 cells were elevated in GBC patients irrespective of clinical stage of patients.Survival analysis showed that Tγδ17, Th17 and Treg cells in peripheral blood were associated with poor survival of GBC patients.

Taken together, our data strongly suggests that Tγδ17 is a pro-tumorigenic subtype of γδT cells andis emerging as a "druggable immune target" that plays an important role in GBC progression.Thus, future immunotherapeutic treatment strategies for GBC may use a combined approach to block the trafficking of Tγδ17 cells to the tumor and inhibit the functions of IL17.

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1. Patil RS, Shah SU, Shrikhande SV, Goel M, Dikshit R, and Chiplunkar SV, “Pro-tumor role of IL17 producing γδT cells in gallbladder cancer”, European Journal of Cancer Volume 54, Supplement 1, Pages S1-S78 (February 2016). doi: 10.1016/S0959-8049(16)31954-2.
2. Patil RS, Shah SU, Shrikhande SV, Goel M, Dikshit R, and Chiplunkar SV, “Role of IL17 producing γδ T cells (Tγδ17) in gall bladder cancer pathogenesis”, Feb10 2015, Journal of Carcinogenesis,14:21.

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171. Name : **Ch. Aminul Islam**
Enrolment No. : PHYS05201004001
Date of Award of degree : 07.02.17
Constituent Institute : Saha Institute of Nuclear Physics,
Title : Study of hot and dense nuclear matter in effective QCD model

Abstract

What we have done to accomplish my thesis is stated briefly in the following few paragraphs. We use various effective QCD models to investigate hot and dense nuclear matter. To characterize such matter we exploit correlation functions and some of the associated spectral properties. In one of the series of works we explore the vector meson current-current correlation function with and without the influence of vector interaction inNambu–Jona-Lasinio (NJL) model and also in its Polyakov loop extended version (PNJL). As a spectral property we have computed the dilepton rate which is found to be enhanced in strongly interacting QGP (sQGP) as compared to the Born rate (leading order perturbative rate) in a weakly coupled QGP. Here the sQGP has been obtained and tuned by the inclusion of a background temporal gauge field, namely the Polyakov loop field. We further consider the idea of entanglement between the chiral and con-finement dynamics through the entangled PNJL (EPNJL) model and re-explore the vector spectral function and the spectral property such as the dilepton pro- duction rate studied in our earlier effort. Because of the strong entanglement between Polyakov loop field and chiral condensate, the coupling strengths run with the temperature and chemical potential. The implications of such running on the dilepton rate have been discussed in details. We also studied, using the aforementioned effective models, the Euclidean vector correlator and the response of the conserved density fluctuations related with the temporal vector correlator. We have considered both the scenarios, i.e. presence and absence of the vector interaction. The inclusion of the vector interaction also brings forth some intriguing issues in the fluctuation of conserved density, namely the QNS. We discuss it in details and try to address it usingEPNJL model. In another effort, we assume the QGP to be made of a non-interacting quarks, antiquarks and gluons and construct a partition function which is restricted by the assumption of a color singlet projection to conform with the SU(3)c symmetry. This projection allows only the color singlet physical states to exist. We showed that this type of simple quantum statistical description exhibits very interesting features: the SU(3)c color singlet has Z(3)c symmetry through the normalized character in the fundamental representation of SU(3)c .This character becomes equivalent to an ensemble of Polyakov loop fields which can be exploited as an order parameter for quark-hadron phase transition.

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2. "Vector meson spectral function and dilepton production rate in a hot and dense medium within an effective QCD approach Chowdhury Aminul Islam, Sarbani Majumder, Najmul Haque and MunshiG. Mustaf JHEP 02 (2015) 011, [arXiv:1411.6407 [hep-ph]].
3. "The consequences of SU (3) colorsingletness, Polyakov Loop and Z(3) symmetry on a quark-gluon gas"Chowdhury Aminul Islam, Raktim Abir, Munshi G. Mustafa, Rajarsh Ray and Sanjay K. Ghosh J. Phys. G 41 (2014) 025001, [arXiv:1208.3146 [hep-ph]].

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172\. Name : **Sanu S. Raj**
Enrolment No. : CHEM01200904003
Date of Award of degree : 9.02.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Synthesis Of Oxide Based Systems: Search For Novel Optical Materials For Radiation Dosimetry

Abstract

The present thesis describes synthesis and characterization of carbon doped oxide materials for radiation dosimetry applications. Fundamental concepts of thermoluminescence (TL) and optically stimulated luminescence (OSL) and their different modes depending upon stimulation and signal detection have been introduced. Detailed discussion has been provided on the defect formation and annihilation mechanism, absorbed dose storage, glow curves and different types of commercially used TL phosphors. Along with the discussion on merits, demerits and current research on the development of new TL and OSL materials, the aim for present work has also been defined. Different synthesis routes employed in this work, such as gel combustion method, have been discussed. Various characterization techniques like powder XRD, TL-OSL-PL setups, and methods adopted for carbon doping have been explained in present thesis. Detailed TL and OSL studies of the $MgAl_2O_4$:C phosphor samples were performed and a decrease in OSL signal was observed with increase in temperature rise as all the TL traps were found to be OSL sensitive. The Computerized Curve De-convolution Analysis (CCDA) has been employed to measure TL parameters such as thermal trap depth, frequency factor and order of kinetic associated with charge transfer process in the TL phenomenon. The photo-ionization cross-section (PIC) associated with fastest OSL component of $MgAl_2O_4$:C is found to be 50% that of the fastest OSL component of commercially available dosimetric grade α-Al_2O_3:C, which is an encouraging result. Photoluminescence study of $MgAl_2O_4$:C synthesized by electron gun and graphite furnace was also performed. It was carried out to analyse the effect of carbon doping on the photo-physical properties of $MgAl_2O_4$. The photoluminescence spectroscopy exhibited defect-induced emissions for both electron gun and graphite furnace sample with enhanced intensity and a significant blue shift in the case of graphite furnace sample. The CIE co-ordinates for graphite sample confirmed it as a blue-light emitter. The multiple trapping and de-trapping events were confirmed by photoluminescence decay studies. The results were complemented by electron paramagnetic resonance (EPR) technique. Detailed studies on the Al_2O_3 nano-powders were also under taken. These samples were synthesized by a fuel-deficient gel combustion synthesis, annealed at different temperatures (1200ºC, 1300ºC, 1450ºC) with the aim of introducing different defect nature/concentration and analyzing their effect on luminescence. At all the three

temperatures, the formation of nano α-Al_2O_3 was revealed by Powder XRD studies. The deconvolution of broad emission spectra yielded three components for all the three samples. These studies helped to understand nature of the defects occurring in Al_2O_3 with the variation in annealing temperatures. These studies provided insights into dosimetry properties of alumina based materials. Thesis concludes with summary and future scope of the work. Carbon doped $MgAl_2O_4$ has exhibited impressive OSL properties, which can be utilized to develop it into a promising phosphor for radiation dosimetry.

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2. Nonlinear-OSL phenomenon defects having closely spaced photoinsation cross-sections in $MgAl_2O_4$:C spinel : D. R. Mishra, Sanu S Raj, A. Soni, K. P. Muthe, S. K. Gupta, M. S. Kulkarni, V. Grover, A. K. Tyagi, Proceedings of the International Conference on Luminescence and its Applications (ICLA- 2012) 7-10th Feb, 2012, Hyderabad, India.

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173. Name : **Vikas Kumar**
Enrolment No. : CHEM01201004011
Date of Award of degree : 9.02.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Synthesis, evaluation and theoretical studies of calix-crown based ligands for cesium recovery from acidic media.

Abstract

Publications

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1. An amide functionalized calix-benzocrown-6 ionophore for the selective extraction of cesium from highly concentrated nitric acid: the e_ect of intramolecular bu_ering, Vikas Kumar, J. N. Sharma, P. V. Achuthan and R. C. Hubli. RSC Adv., m2014, 4, 805-810.

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174. Name : **Alok Kumar Saxena**
Enrolment No. : PHYS01201004001
Date of Award of degree : 9.02.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Optimization Of Electric Gun Setup To Study Shock Responses Of Zr And Ti.

Abstract

The present research discusses about the development and optimization of an experimental facility to study the high pressure dynamic behavior of various metals. Zirconium and titanium are considered for present study as these metals and their alloys are of great importance for nuclear reactor as well as nuclear waste managements programs due to their high corrosion resistance and low neutron interaction cross-section. The alpha to omega phase transition in these metals is the topic of scientific interest due to dependence of transition pressure on various material properties and experimental parameters including pressure exposure time. The present study reports phase transitions and shock studies on thin foils where pressure pulse duration is relatively small and can be controlled by experimental parameters. The development of optical diagnostics for accurate shock research is also an important part of this work. A single beam Fabry-Perot

Velocimeter (FPV) developed earlier has been modified and improved to simultaneously measure two velocity profiles using a single laser and streak camera. This improvement in FPV makes shock diagnostics more accurate, economic and operationally simple. The design details and error analysis of Fabry-Perot velocimeter records are described in the thesis.A portable electric gun setup of 8 kJ energy has been developed as a projectile launcher for generating shock pulses up to 70 GPa pressure in materials like tantalum. As the projectile velocity depends on various interrelated experimental parameters, effect of design parameters like foil dimensions, barrel diameter, its length and pressure of surrounding medium on flyer velocity has been experimentally investigated. The concept of flyer velocity enhancement by compressed plasma propulsion is conceived and experimentally implemented to achieve velocities up to 4.5 km/s on small diameter (6mm) aluminum flyers and 6.3 km/s on polyimide flyers. A concept of two stage exploding foil assemblies has been experimentally explored, where fast explosion of metallic foils is achieved by steepening the current pulse using an opening switch in the first stage. For better understanding of electric gun performance, an earlier developed one dimensional hydrodynamic numerical scheme has been suitably modified and implemented to numerically simulate the flyer velocity profiles. The performance of this numerical scheme is validated against experimental and simulation data reported in literature on such systems. Numerically computed flyer velocity profiles and final flyer velocities have been found to be in close agreement with the experimental results measured on our system as well as reported elsewhere in literature.Shock experiments were carried using single beam velocimeter on different metals like tin, iron, titanium, tantalum, aluminum etc. up to pressures of typically 50- 70 GPa. The phase transition in iron from bcc to hcp phase has been *in situ* recorded at 13.6 GPa pressure using single beam FPV. More precise EOS measurements were carried using dual beam velocimeter on zirconium and titanium metals up to pressures of 12 GPa and 16 GPa respectively. The detailed velocity profiles of target-glass interface show a weak kink in its rising part indicating a phase transition from α phase to ω phase. The transition pressure in present study is found to be approximately 8.2 GPa for zirconium and 11.4 GPa for titanium, which are quite in agreement with the values reported in literature on thicker samples of similar impurity concentrations.

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6. A. K. Saxena, A. C. Jaiswar and T. C. Kaushik, " A low cost optically isolated setup for DC high voltage measurements," *Proc. of 29th National Symposium on Plasma Science & Technology (PLASMA 2014), Mahatma Gandhi University, Kottayam,* Kerala, India, p.342 (2014).

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175. Name : **Jayaraj**
Enrolment No. : ENGG01201104003
Date of Award of degree : 10.02.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Investigation On The Natural Circulation Characteristics Of A Molten Salt Loop.

Abstract

High Temperature Reactors (HTR) and solar thermal power plants use molten salts as a coolant/heat transfer fluid. Molten salts have comparatively low melting point and high boiling point at low pressure. This is highly desirable because a high temperature system can be designed without increasing system pressure. Hence design and operation of molten salt based system gets simplified. Natural circulation of molten salt is being preferred in some systems like solar thermal power plant or molten salt fast breeder reactor. Such systems can be studied with the help of a natural circulation loop. Natural circulation loops are representative of primary heat transport system of nuclear reactor and other facilities working on natural circulation flow. A Natural Circulation Loop (NCL) consists of a heater and cooler connected by piping. The heater is placed at lower elevation than the cooler. As a consequence of the heat flux, the heated part of the fluid becomes lighter and rises up, while the cooler part becomes denser and drops down due to gravity. These combined effects establish natural circulation of fluid in the loop. Thus, the motive force for the flow in NCL is generated simply because of the presence of the heat source and heat sink, without need of any external force. The absence of moving/rotating parts to generate the motive force for flow makes it less prone to failures. Also maintenance and operating costs are reduced. Hence the heat removal/transfer by natural circulation system takes the most attention. In view of this, molten salt natural circulation loop has been installed to study heat transfer capability of molten salt and also to understand the steady state and transient thermal-hydraulic behaviour of molten salt natural circulation loop. Experimental and computational investigations of natural circulation loop with water are published previously. These available experimental data are used to understand the thermal-hydraulic behaviour of natural circulation loop working with water. Hence, the rectangular natural circulation loop working with water is also simulated using 3D CFD software. The CFD results are compared with available experimental data and correlations to validate the CFD models. The promising results obtained from CFD simulation are used to explain the reason behind the uni-directional and bi-directional oscillations occurs in the horizontal cooler and horizontal heater configurations of the natural circulation loop. This is one of the novel contributions of this thesis.Transient 3D CFD simulation of the molten salt natural circulation loop is carried out. The experimental data generated on molten salt natural circulation loop are used to validate the CFD model, whereas the computed data are useful to know the design parameter of molten salt reactor and also for solar power plant. Various transient

computational studies such as (i) flow initiation transients, (ii) power rising from steady state transients, (iii) power step back transients, (iv) heater trip transients and (v) loss of heat sink transients are performed to understand the thermal-hydraulic behavior of the loop at different operating conditions and various orientations of heater and cooler. Further, the heat transfer study on molten salt natural circulation loop has been carried out. The steady state heat transfer characteristics shows good match with Boelter's mixed convection correlation. Effect of developing length on heat transfer has been studied. The transient unsteady heat transfer characteristics are also studied and the unique heat transfer characteristic in the oscillatory flow has been explained in the thesis.

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3. A. K. Srivastava, Jayaraj Y. Kudariyawar, A. Borgohain, N. K. Maheshwari and P. K. Vijayan, Experimental and theoretical studies on the natural circulation behaviour of molten salt, Applied Thermal Engineering, 98 (2016), 513-521. http://dx.doi.org/doi:10.1016/j.applthermaleng.2015.12.065
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176. Name : **Nidhi Garg**
Enrolment No. : CHEM01201104021
Date of Award of degree : 14.02.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Preparation And Characterization Of Zirconia Coatings On Stainless Steel Developed By Hydrothermal Process.

Abstract

Stress corrosion cracking (SCC) of the structural components fabricated of type 304/304L/304LN stainless steel (SS) is a critical issue for the structural integrity of boiling water reactors (BWRs). SCC problem is also expected in future advanced heavy water reactors (AHWRs) because of the use of type 304LN SS as the structural material and its coolant water chemistry being similar to BWR. Hydrogen water chemistry (HWC) and noble metal chemical addition (NMCA) are the most widely used techniques for mitigation of SCC in nuclear reactors. But these techniques are not suitable to provide protection at certain locations of structural materials. In addition, HWC technology leads to significant increase of radiation dose in main steam line. To get rid of these drawbacks, inhibitive protective coating of zirconia on SS surface is proposed to mitigate the SCC problem. The insulating nature of the zirconia inhibits the redox reactions at the surface by cutting off the electrical connection between oxidants in water and the metal components. Hydrothermal method is the only applicable method for industrial scale deposition of zirconia on SS surface. Two methods of zirconia deposition on SS by hydrothermal process are presented in this thesis. The first one is adsorption of nano-zirconia on pre-oxidized SS surfaces. Adsorption of nano-zirconia on pre-oxidized SS surfaces was carried out in aqueous solution at different temperatures. Although this method led to the deposition of nano-zirconia on SS surface, but did not provide a full substrate surface coverage. The second method involves the deposition of zirconia in a static autoclave by using aqueous solution containing ZrO(NO3)2.6H2O salt, Na-EDTA (disodium salt dehydrate) and sodium dodecyl sulphate (SDS). This method was found tobe promising and led to deposition of continuous, tetragonal nano-zirconia coating on pre-oxidized SS surfaces. Intermediate SS surface oxide layer (also termed as pre-oxidized layer) is necessary to deposit adherent zirconia coating on SS surface. Chemical composition, oxide particle size and morphology of the pre-oxidized SS surface influence the zirconia coating properties like adhesion, continuity and thickness. The pre-oxidized SS specimens with different chemical compositions and surface morphologies are prepared. SS surfaces pre-oxidized in a static autoclave in reducing water chemistry environment showed the formation of spinel oxides like ferrites and chromites. The pre-oxidized SS specimens prepared in static autoclave in normal water showed that the surface oxide layer is composed of rhombohedral oxides like -Fe2O3, -Fe2-xCrxO3 and spinel oxides. To prepare stoichiometric α-Fe2O3 on SS surface, pure α-Fe2O3 films were developed on stainless steel surface by pulsed laser deposition technique. Deposited α-Fe2O3 particles were spherical and uniform in size. SS surface composed of -Fe2O3 was found to be the most suitable for continuous and thick zirconia coating while the pre-oxidized layer composed of spinel oxides resulted in thin and discontinuous coating. The mechanism of the growth of zirconia on the most favorable surface oxide (-Fe2O3) has been explored. It is shown that Na salt of Zr-EDTA is formed in the solution prior to the interaction of Zr-precursor with the pre-oxidized surface. Interaction of Na salt of Zr-EDTA with α-Fe2O3 surface resulted in the formation of metastable Fe2O3-ZrO2 compositions at around 200oC which provided the suitable interface for the growth of tetragonal ZrO2 coating. X-ray photoelectron spectroscopy studies established the formation of Fe-O-Zr bonding states at the interface. ZrO2 particles grew in the form of islands on the α-Fe2O3 surface at the initial stage and these islands grew and coalesce to form the

continuous and thick coating. iii the electrochemical properties of the zirconia coated SS samples have been studied with respect to the pre-oxidized SS specimens and plain SS at different temperatures. The coating developed over spinel oxide surface was porous, discontinuous and could not act as an insulated barrier. Still it showed improvement in the corrosion resistance compared to the uncoated surface. Zirconia coating developed over nano -Fe2O3 showed the best corrosion resistance, lowest porosity and insulating barrier like characteristics. Nano-mechanical properties like adhesion, hardness at nano-scale using atomic force acoustic microscopy and force-distance spectroscopy are discussed. Grains and grain boundaries of the zirconia coating showed the significant impact on corrosion resistance and hardness. The substrate surface morphology plays major role in deciding the adhesion, thickness and compactness of ZrO2 coatings. Small particle size and hills/valley type morphology of the pulsed laser deposited α-Fe2O3 films provide large surface area for interaction with Na salt of Zr-EDTA during the hydrothermal process which improves the adhesion. Thickness of ZrO2 coatings are improved by multiple repetitions of hydrothermal deposition process with fresh reactants. Multiple rounds of deposition of ZrO2 coating on the pre-oxidized SS surface led to the improvement of coating thickness from 200 nm to ~1.2 m after four repetitions. Corrosion resistance of the ZrO2 coated samples at room temperature increased remarkably with the increase in thickness and stabilized after third repetition where coating thickness was around 1 m. Electrochemical measurements like potentiodynamic polarization test and electrochemical impedance spectroscopy are used for the optimization of ZrO2 coating thickness for corrosion resistance applications.

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2. “Role of chemical composition of oxide layer on stainless steel for ZrO2 coating by hydrothermal process”, Nidhi Garg, Vinit K Mittal, Santanu Bera, P. Chandramohan, C.R. Das, S. Velmurugan, Thin Solid Films, 2013, 545, 222-228.
3. “Study of Fe2O3-ZrO2 interface of ZrO2 coating grown by hydrothermal process on stainless steel”, Nidhi Garg, Santanu Bera, G. Mangamma, Vinit K Mittal, R. Krishnan, S. Velmurugan, Surface and Coatings Technology, 2014, 258, 597-604.
4. “Electrochemical and adhesion properties of hydrothermally deposited nano-ZrO2 coatings on oxide layers of stainless steel”, Nidhi Garg, Santanu Bera, G. Mangamma, C.R. Das, S. Kamaruddin, S. Velmurugan, Surface and Coatings Technology, 2015, 281, 98-108.

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177. Name : **Rajan Kumar Choudhary**
Enrolment No. : LIFE09201004019
Date of Award of degree : 14.02.17
Constituent Institute : Tata Memorial Centre
Title : Molecular Mechanism of BRCA1-BARD1-CstF50 Complex and Breast Cancer Risk.

Abstract

BRCA1-BARD1 E3 ubiquitin ligase and CstF50 protein-protein complex plays an important role in transcription coupled DNA damage repair. Germ-line mutations identified in BARD1 ARD-BRCT linker region at Gln564His position impairs the complex formation between BARD1 and CstF50, which in turn leads to premature transcript formation, uncontrolled mRNA regulation and reduced apoptosis. Biophysical and in-vitro assay could unravel the changes in folding pattern and structuralintegrity of the BARD1 *wild-type*andGln564His mutant protein. Molecular docking studies of CstF50 with BARD1 *wild-type* and mutant show loss of weak intermolecular interactionsin mutant protein. Molecular Dynamics simulation shows that mutant protein is more dynamic in nature compared to *wild-type* protein.It has been observed that the C-terminal domain of BARD1 is evolutionarily conserved phosphopeptide binding domain and have a wide role in DNA damage repair (DDR) and cell-cycle regulation. Cancer predisposing mutations C645R, R658C,V695L, I738V and S761N are reported in BARD1BRCT domain. Thermal and chemical denaturation studies reveal decrease in the thermodynamic stability of BARD1V695L, S761N, R658C and I738V mutants than the *wild-type,* and all proteins unfold via intermediate formation. Molecular Dynamics simulation studies of*wild-type* and mutant protein structures indicate that the mutants have lost structural integrity compared to the *wild-type* protein. We are alsodescribing the inhibitory effect of platinum drug on E3 ubiquitin ligase activity of BRCA1-BARD1 Ring domain complex. The docking study betweenplatinum drug and BRCA1 Ring domain shows the overlapping of platinum drug binding site with E2 ligase binding site;this concludes that platinum drug may interfere with E2 binding. Multidisciplinary comparative studies ofBARD1 *wild-type* and mutants will be helpful in understanding the role of BARD1BRCT in DDR, cell-cycle regulation and tumorigenesis.

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2. Functional basis and biophysical approaches to characterize the C-terminal domain of human-Ribosomal s6 Kinase 3. Bhanu P. Jagilinki,Rajan Kumar Choudhary, Pankaj S Thapa, Nikhil Gadewal,M.V.Hosur, Satish Kumar, Ashok K Varma, Cell Biochemistry & Biophysics, June, 2016, pp 1-9, doi:10.1007/s12013-016-0745-6.

Conferences attended:

1. Indian Association for Cancer Research (IACR), ACTREC, 26-29 January, 2012,.
2. 2nd Global Cancer Genomics Symposium (GCGC), ACTREC, 19-20th November, 2012
3. International Conference on Structural Genomics 2015 – Deep Sequencing Meets Structural Biology (ICSG2015-DSMSB), Weizmann Institute of Science, Rehovot, Israel,7-11 June, 2015

178. Name : **Shalik Ram Joshi**
Enrolment No. : PHYS07201004004
Date of Award of degree : 23.02.17
Constituent Institute : Institute of Physics,
Title : Nanostructure Formation on Rutile TiO2 and Ta surfaces by Ion Beam Irradiation : Photoabsorption, Magnetism, Scaling and KMC Studies.

Abstract

The present thesis discusses the generation of nano-patterns on single crystal semiconducting rutile TiO_2 surfaces and metallic Tantalum surfaces via the technique of ion irradiation. In both the cases the nanostructures are generated through the competition between the erosion and diffusion processes. The scaling studies on these non-equilibrium surfaces as well as the scaling exponents show that these surfaces belong to different universal classes. Results presented here further show that the inclusion of Schwoebel barrier in the metallic tantalum is important for understanding pattern formation. On the TiO_2(110) surface, preferential sputtering of oxygen atoms leads to the formation of Ti rich zones that become the nucleation sites for the development of nanostructures. The results show an enhanced photo absorption from these nano-patterned surfaces. Development of nanostructures on the surface and creation of vacancy sites along with the formation of $Ti_{1-x}Co_xO_2$, $CoTiO_3$ and Co nanoclusters, upon ion irradiation, promote the high photo absorption and the reduced band gaps observed here. Formation of the cobalt nanoclusters, after implantation, also manifests in unusual superparamagnetic properties in this system. The observed SPM is in-equivalent along the two crystallographic axes of the TiO_2 lattice as demonstrated by the behaviour of magnetic moments, above and below the blocking temperature. Scaling studies above blocking temperature also display this anisotropy. Presence of nanoclusters, with dipole dipole interactions and inter-cluster exchange interactions, produce these anisotropies. RBS/C results also display presence of these Cobalt-clusters along with an increase in depth dependent damage below the surface. Multiple scattering formalism has been applied to obtain the depth dependent damage profiles which indicate dynamical annealing of defects at the End-of-range. Scaling studies of TiO_2 surfaces, based on the non-equilibrium growth models, indicate that these surfaces after irradiation belong to the EW class. In the nano patterns created on the metallic Tantalum surfaces, Schwoebel barrier plays an important role as has been demonstrated here through 1+1 dimensional KMC simulations. The Schwoebel effect has been incorporated here via a weak non linearity in the Hamiltonian. Comparison of simulations with experimental results show that the morphology of ion irradiated Tantalum surfaces belongs to a universality class other than EW and KPZ.

Publications

Journal

1) *Effect of Cobalt Implantation on Structural and Optical Properties of Rutile TiO_2(110), Shalik Ram Joshi, B. Padmanabhan, Anupama Chanda, V. K. Malik, N. C. Mishra, D. Kanjilal and Shikha Varma, Applied Physics A, 122, 713, (2016).
2) *Optical Studies of Cobalt Implanted Rutile TiO_2(110) Surface, Shalik Ram Joshi, B. Padmanabhan, Anupama Chanda, Indrani Mishra, V. K. Malik, N. C. Mishra, D. Kanjilal and Shikha Varma, Applied Surface Science, 387, 938-943 (2016).
3) *Kinetic Monte Carlo Simulations of Self Organized Nanostructures on Tantalum Surface Fabricated by Low Energy Ion Sputtering, Shalik Ram Joshi, Trilochan Bagarti and Shikha Varma, Surface Science 641, 170-173 (2015).
4) Ion-beam-induced nanodots formation from Au/Si thin films on quartz surface, D.P. Datta, V. Siva, A. Singh, Shalik Ram Joshi, D. Kanjilal, P.K. Sahoo, Nuclear Instruments and Methods in Physics Research B, 379, 48-51, (2015).

5) Room Temperature Superparamagnetism in Rutile TiO_2 Quantum Dots Produced Via ECR Sputtering , Vanaraj Solanki, Indrani Mishra, Shalik Ram Joshi, P. Mishra, P. Dash, N. C. Sharma, Dinakar Kanjilal and Shikha Varma, Nuclear Instruments and Methods in Physics Research B 365, 82-85 (2015).
6) Size-dependent optical properties of TiO_2 nanostructures, Vanaraj Solanki, Subrata Majumder, Indrani Mishra, Shalik Ram Joshi, Dinakar Kanjilal and Shikha Varma, Radiation Effects and Defects in Solids 168, 518-524 (2013).
7) Oxygen vacancy mediated enhanced photo-absorption from ZnO(0001) nanostructures fabricated by atom beam sputtering, Vanaraj Solanki, Shalik Ram Joshi, N.C. Mishra, D.K. Awasthi and Shikha Varma, Journal of Applied Physics, 120, 054303, (2016).
8) Scaling Studies of Nanopatterned TiO_2 (110) Surfaces Created via Low Energy Ion Irradiation, Indrani Mishra, Shalik Ram Joshi, S. Majumder, Ashis Kumar Manna and Shikha Varma, Radiation Effects and Defects in Solids, (DOI: 10.1080/10420150.2016.1225067).
9) Effect of Self Affine Morphology of Natively oxidised Silicon(100) on Wetting, Scaling Properties and DNA Fractal Dimension, Indrani Mishra, Shalik Ram Joshi, Subrata Majumder, U. Subudhi and Shikha Varma, (Under Review).
10) Conducting Polymer PEDOT:PSS: An Emerging Material, Anupama Chanda, Shalik Ram Joshi, Rakesh Sahoo, Shikha Varma, Kwangsoo No, (Under Review).
11) *Unusual Superparamagnetism in Cobalt Implanted Rutile TiO_2 (110), Shalik Ram Joshi, B. Padmanabhan, Anupama Chanda, Neeraj Shukla, V. K. Malik, D. Kanjilal and Shikha Varma, (Under Review).
12) *Damage Studies of Cobalt Implanted Rutile TiO_2 (110) Lattice via. RBS/C, Shalik Ram Joshi, B. Padmanabhan, Anupama Chanda, V. K. Malik, S. Ojha, D. Kanjilal and Shikha Varma, (Under Review).
13) *Scaling Studies of Self Affine Nanostructures on TiO_2 (110) surfaces via. Ion Irradiation, Shalik Ram Joshi, Anupama Chanda, D. Kanjilal and Shikha Varma, (Under Review).
14) Photoabsorbance Properties of Constrained Nanostructures on Rutile TiO_2 (110) Surface, Vanaraj Solanki, Shalik Ram Joshi, Indrani Mishra, Dinakar Kanjilal and Shikha Varma, (to be submitted).

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179. Name : **Subikash Choudhury**
Enrolment No. : PHYS04201004006
Date of Award of degree : 23.02.17
Constituent Institute : Institute of Physics,
Title : Di-hadron correlations with identified leading hadrons at intermediate transverse momentum in Pb-Pb 2.76 TeV in ALICE.

Abstract

Exploring the mechanism of particle productions at intermediate transverse momentum (pT) , 2< pT< 5 GeV/c has been the main objective of my thesis. An unusually enhanced baryon generation over meson reported for the first time at the RHIC heavy ion program had not been predicted earlier by any of the established models until it was observed experimentally. A succinct explanation to theobserved anomaly was offered by the models invoking hadronization via recombination or coalescence of quarks. The constituent quark number (ncq) scaling observed in the measurements of elliptic flow coefficients of different hadrons is a suggestive of coalescence being a plausible mechanism of hadronformation at intermediate pT .Since then lot of theoretical investigations have been pursued to unveil the enigma of particle production at moderate pT . In my thesis work I have adopted the technique of two-particle correlations to probe whether correlation strength is sensitive to the coalescence formalism. To quantify the effect, I have calculated the near side jet-like yield associated with baryon-hadron and meson-hadroncorrelations. Baryons generation being favoured in coalescence formalism, a naive expectation would be, a suppressed baryon trigger yield as it is unlikely to have correlated partners at small angles forthe particle produced by quark coalescence. I have explicitly look for this signature in data and Monte Carlo event generators that implements coalescence as a mode of hadronization.

Development of Resistive Plate Chamber (RPC) for high energy physics experiments

Resistive Plate Chamber (RPC) is a gas-based detector made of highly resistive materials like glass or High Pressure Laminate (HPL), better known as bakelite. Excellent time resolution (0.5 ns), large surface area and relatively low-cost makes RPC best-choice for triggering and muon detection in high energy experiments. A large size (240 cm × 120 cm × 0.2 cm) oil-free bakelite Resistive Plate Chamber (RPC) has been fabricated at VECC-Kolkata using locally available P-302 OLTC grade HPL . The chamber has been subjected to streamer mode of operation using Argon, Freon(R134a) and Iso-butane in a ratio of 34:57:9 by volume. The performance of the chamber has been characterized by measuring the long term efficiency, its uniformity and stability against the variation of humidity and temperature by detecting the cosmic muons. Timing measurement has been performed at a central location of the chamber. The chamber maintained an efficiency of ≈ 95% and time resolution at the point of measurement, 0.83 ns at 9000V over a period of 30 days at the time of writing this thesis.

Publications

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1. “Effect of radial flow on two particle correlations with identified triggers at intermediate pTin p-Pb collisions at 5.02 TeV”, Debojit Sarkar, Subikash Choudhury, Subhasis Chattopadhyay, Physics Letters B, pp. 763-768 (2016).
2. “Testing of the coalescence mechanism in high energy heavy ion collisions using two-particlecorrelations with identified particle trigger”Subikash Choudhury, Debojit Sarkar, Subhasis Chattopadhyay ,Phys. Rev. C 93, 054902 (2016).
3. “ Present and future of QGP research in high energy heavy ion collisioexperiments”Subhasis Chattopadhyay, Subikash Choudhury, Debojit Sarkar,Indian Natn Sci Acad 81(2015)321-335.
4. “ Two particle correlations with identified at intermediate pT with identified leading hadrons atthe LHC energy using AMPT model”Subikash Choudhury, Debojit Sarkar, Subhasis Chattopadhyay,Springer Proceedings in Physics, XXI DAE-BRNS, High Energy Physics Symoposium Proceedings.
5. “Fluctuations in Charged Particle Multiplicities in Relativistic Heavy-Ion Collisions”,Maitreyee Mukherjee, Sumit Basu, Subikash Choudhury, Tapan K. Nayak, J. Phys. G: Nucl. Part. Phys. 43, 085102 (2016).
6. “Fabrication and Characterisation of Oil-Free Large High Pressure Laminate Resistive PlateChamber”, Rajesh Ganai, Arindam Roy, Kshitij Agarwal, Zubayer Ahammed, Subikash Choudhury, Subhasis Chattopadhyay, JINST 11 P04026, (2016).

180. Name : **Suman Gupta**
Enrolment No. : ENGG02200904009
Date of Award of degree : 23.02.17
Constituent Institute : Indira Gandhi Centre for Atomic Research,,
Title : Investigation On Structural Mechanics Coupling Of Perforated And Unperforated Thick Tube Sheet For Sodium To Sodium Heat Exchanger

Abstract

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181. Name : **E. Prabhu**
Enrolment No. : CHEM02200804013
Date of Award of degree : 23.02.17
Constituent Institute : Indira Gandhi Centre for Atomic Research,,
Title : Studies On The Characteristics Of In2o3, Ag6mo10o33and Pd Based Materials Towards Sensing Different Gaseous Species.

Abstract

Large quantities of hazardous gases like NO, NO_2, SO_2, H_2S and NH_3 are handled in industrial processes and accidental release of these gases to ambient air will lead to severe pollution. In addition, H_2, and NH_3 can form explosive mixtures with oxygen in air and lead to undesirable consequences. The objective of the thesis is to understand the sensing characteristics of certain select materials towards target analytes. Thesis focused on the sensing mechanism of indium oxide as thin film towards NO_X (mixture of NO & NO_2) using van der Pauw, and Hall measurement between the temperature of 373 and 673 K. Using these techniques, change in four probe conductivity, carrier concentration and mobility of the thin film in air and air containing NO_X was measured. Products like (NO_3^-), $(NO)_2^{2-}$ and $(NO_2)^-$ were identified using laser Raman and it was established that these products are responsible for change in carrier concentration, conductivity and mobility of the In_2O_3 at different temperatures. Among various oxides, $CuInO_2$ (p-type) and $Cu_2In_2O_5$ (n-type) were tested for their sensing behavior with the analytes. As $CuInO_2$ is a metastable compound, it was prepared as thin film using PLD in controlled oxygen pressure. The thin film of $CuInO_2$ showed excellent selectivity towards NO_X at 473 K. But $Cu_2In_2O_5$ showed cross sensitivity to the gases investigated. Studies on identification of palladium based alloys for sensing hydrogen at 300 K in argon were undertaken. Conditions for the preparation of nano palladium, nickel substituted palladium ($Pd_{1-X}Ni_X$ [x = 0, 0.05 & 0.1]) and cobalt and nickel substituted palladium ($Pd_{1-X-Y}Ni_XCo_Y$ [x = y = 0.05]) using low temperature reduction technique were optimized. The sensitivity of alloy thin films was found to increase with the nickel concentration in palladium in $Pd_{0.97}Ni_{0.03}$ and $Pd_{0.93}Ni_{0.07}$. On the other hand, sensitivity of $Pd_{0.91}Ni_{0.04}Co_{0.05}$ thin film showed marginally higher sensitivity towards hydrogen than palladium. Silver decamolybdate, $Ag_6Mo_{10}O_{33}$ was recognized as a good material for sensing trace levels of NH_3 by the earlier studies. It possessed significant Ag^+ conductivity. However, measuring its electrical resistivity by two probe DC led to polarization due to steady transport of silver between the electrodes and drift in the sensor output. Thesis described the incorporation of tungsten in silver molybdates [$Ag_6Mo_{10-X}W_XO_{33}$ (X = 0 – 2.0)] to understand the electrical properties. The nominal compositions, $Ag_6Mo_{9.75}W_{0.25}O_{33}$ and $Ag_6Mo_{9.5}W_{0.5}O_{33}$ showed better enhanced conductivity than $Ag_6Mo_{10}O_{33}$. AC impedance studies of $Ag_6Mo_{10}O_{33}$ thick film showed promising selectivity towards NH_3 at 573 K without drift in the thick film baseline.

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Journal

1. ‘‘Changes in carrier concentration and Debye length: Experimental evidence fromvan der Pauw Hall Measurements on NOX sensing of In2O3”E. Prabhu , K.I. Gnanasekar, T.R.Ravindran, V. Jayaraman and T. Gnanasekaran, J. Electrochem. Soc., 169 (2014) B1 – B7.
2. “Preparation, characterization and NOX sensing characteristics of sensor gradeCuInO2 thin films”E. Prabhu, K.I. Gnanasekar, V. Jayaraman, and T. Gnanasekaran, Mat.Sci. Forum710, (2012) 727 – 732.
3. “Structural, electrical conductivity and transport studies on Ag6Mo10-XWXO33 (X = 0– 1) – A class of silver ion conductors”E. Prabhu, K.I. Gnanasekar, V. Jayaraman and T. Gnanasekaran,J. Electrochem. Soc., 2015 (Under Review)
4. “Low temperature synthesis of metals and alloys of palladium and their hydrogeninteraction behavior in argon”E. Prabhu, K.I. Gnanasekar, V. Jayaraman and T. Gnanasekaran.Int. J. Hydrogen Energy, 2015 (Manuscript under preparation)
5. “Analysis of Nano-structured In2O3 thin film NOX sensor by AC impedancespectroscopy”C.R. Mariappan, E. Prabhu, K.I. Gnanasekar, V. Jayaraman & T. Gnanasekaran,IEEE Sensors 14, 3, (2014) 651 – 656v

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182. Name : **Milan Kr. Barman**
Enrolment No. : CHEM11201004014
Date of Award of degree : 23.02.17
Constituent Institute : National Institute of Science Education and Research,
Title : Bulky Guanidinate Ligand Stabilized Main Group Metal Complexes: Synthesis, Characterization and Reactivity Studies.

Abstract

The general formulaof guanidines is $R_1–N=C(NR_2R_3)NR_4R_5$, in which the carbon atomof the N_3C functional group is connected to one imino and twoamino nitrogen atoms.In 1970, Lappert and coworkers reported the first transitionmetal guanidinate complex. Since then, a large number ofguanidinate supported coordination complexes involving metalsfrom across the periodic table have been described. In recentyears, the chemistry of guanidinate stabilized low oxidation statemetal complexes with metal-metal (single or multiple bonded) or metal with non-bonded electrons both are the emerging area.To isolate such unusual molecules the utilization of bulky guanidineligand systems are very important, because these can provide stericand/or electronic protection from processes such as disproportionation,oligomerization etc. Therefore, by employing bulky guanidine ligand a series of s- and p- block metal complexes have been reported. Mainly, this thesis describes well defined main group metal complexes bearing bulky guanidinate ligands. Further, their reactivity studies and as precatalysts for organic transformations have been discussed.This thesis consist of six chapters, 1st chapter comprises general introduction of guanidinine ligand and literature survey of important main group molecules bearing guanidine ligand. Chapter 2 describes synthesis,characterization and catalytic activity of homoleptic and heterolepticMg(II), Ca(II) and Zn(II) complexes. Chapter 3 reveals guanidinato magnesium amides as catalysts for the hydroboration of ester and mixed metal amides bearing guanidine ligand. Chapter 4 contains guanidinato aluminium amide complexes used as catalyst for Tischenko reaction. Chapter 5 describes guanidinato low valent Ge(II) and Sn(II) amide complexes and their reactivity studies. And finally in last chapter, synthesis and characterization of group 14 homoleptic metallynes and their oxidative additions with chalcogens.

Publications

Journal

1. AshimBaishya, V RaoMundlapati, SharanappaNembenna* and Himansu S Biswal*, Structure, bonding and energetics of N-heterocyclic carbene (NHC) stabilized low oxidation state Group 2 (Be, Mg, Ca, Sr and Ba) metal complexes: A theoretical study, *Journal of Chemical Sciences*, 2014, *126*, 6, 1781-1788.
2. AshimBaishya, Milan Kr. Barman, ThotaPeddarao, SharanappaNembenna*, Catalytic C–N bond formation in guanylation reaction by N-heterocyclic carbene supported magnesium(II) and zinc(II) amide complexes, *Journal of Organometallic Chemistry,* 2014,*769*, 112-118.
3. AshimBaishya, ThotaPeddarao, Milan Kr. Barman and SharanappaNembenna*, Catalyst free C–N bond formation by the reaction of amines with diimides: bulky guanidines*, New Journal of Chemistry,* 2015, *39*, 7503-7510,
4. AshimBaishya, Lokesh Kumar, Milan Kr. Barman, ThotaPeddarao andSharanappaNembenna*, Air stable N-heterocyclic carbene-carbodiimide (“NHC-CDI”) adducts: bulky amidinates,*ChemistrySelect,* 2016, *3*, 498-503.

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183. Name	:	**Tapas Kumar Achar**
Enrolment No.	:	CHEM11201004010
Date of Award of degree	:	23.02.17
Constituent Institute	:	National Institute of Science Education and Research,
Title	:	Enabling Non-Conventional Pathway for Organic Synthesis.

Abstract

In recent times, chemists have put sincere efforts to develop methods to use alternative energy as a source of energy-input for chemical transformations. Therefore, non-conventional energy sources, such as microwave, ultrasound, mechanical grinding and visible light are becoming popular. In addition, minimizing waste and developing recyclable methodology is an important aspect for doing chemical synthesis in a greener fashion. Main objective of this thesis is to develop more viable and efficient synthetic protocols using ball milling and ultrasound.This thesis has been organized in five chapters. In chapter-1, we have discussed brief historical overview and mechanistic aspects of mechanochemistry. Chapter-2 represents the efficiency and synthetic utility of 2-iodoxybenzoic acid (IBX) under solvent free milling conditions. A solvent and metal-free cross-coupling method for oxidative amidation of aldehydes and alcohols has been demonstrated in Chapter 3. Chapter-4 describes a method to transform an explosive mixture into a successfulcross dehydrogenative coupling (CDC) reaction for synthesis of amides at extreme conditions. In chapter-5, we have discussed mechanoresponsivity of small benzocyclobutenols which is controlled via intra-molecularly as well as intermolecular effects like solvent polarity and supramolecular interactions.

Publications

Journal

1. Achar, T. K.; Maiti, S.; Mal, P. PIDA-I_2 mediated direct vicinal difunctionalization of olefins: iodoazidation, iodoetherification and iodoacyloxylation. *Org. Biomol. Chem.*2016, *14*, 4654-4663.

2. Achar, T. K.; Mal, P. Transformation of Contact-Explosives Primary Amines and Iodine(III) into a Successful Chemical Reaction under Solvent-Free Ball Milling Conditions. *Adv. Synth. Catal.*2015, *357*, 3977-3985.
3. Achar, T. K.; Mal, P. Radical-Induced Metal and Solvent-Free Cross-Coupling Using TBAI–TBHP: Oxidative Amidation of Aldehydes and Alcohols with N-Chloramines via C–H Activation. *J. Org. Chem.*2015, *80*, 666-672.
4. Achar, T. K.; Maiti, S.; Mal, P. IBX works efficiently under solvent free conditions in ball milling. *RSC Adv.*2014, *4*, 12834-12839.
5. Achar, T. K.; Prakash, V.; Biswal, H. S.; Mal, P. An isoquinoline as cation assisted ON–OFF–ON fluorescence switch with methionine and fluoride ion. *Tetrahedron Lett.*2013, *54*, 1067-1070.

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184. Name : **Prasit Kumar Sahoo**
Enrolment No. : CHEM11201104005
Date of Award of degree : 23.02.17
Constituent Institute : National Institute of Science Education and Research,
Title : Subcomponent Synthesis via Mechanochemistry.

Abstract

Mechanochemistry (solvent-free ball-milling) has gained substantial interest due to its advantages over traditional solution-based methods. Mechanochemical Synthesis is generally time saving, environmental friendly and economical. However, the subcomponent self-assembly approach under system chemistry, is a method in which ligands of metallo-supramolecular complexes are produced in situ from their subcomponents. With rising public concern over alternative energy and global warming, it is important to decrease the usage of chemicals in routine chemical synthesis. Essentially, developing recyclable methodology and eliminating waste are important parts of chemical reactions. Therefore organic synthesis using subcomponent technique under mechano-milling is a useful tool for doing chemical reaction in a greener fashion.Recently, ball-milling is used for synthetic transformations due to its benefits over solution based methods. Many advantages are associated during synthesis by mechanochemistry. This method has huge importance for green processes due to time efficiency, environmentally friendliness and inexpensive synthesis. In this thesis, attempts have been made to show that day by day use of ball-milling become superior tool over solution based conventional method.

Publications

Journal

1. P. K. Sahoo, A. Bose; P. Mal, Solvent-Free Ball-Milling Biginelli Reaction by Subcomponent Synthesis. *Eur. J. Org. Chem.*2015, *32*, 6994
2. C. Giri,* P. K. Sahoo,* R. Puttreddy, K. Rissanen, P. Mal, Solvent-Free Ball-Milling Subcomponent Synthesis of Metallosupramolecular Complexes. *Chem. Eur. J.,*2015, *21*, 6390 (*contributed equally)
3. P. K. Sahoo, C. Giri, T. S. Haldar, R. Puttreddy, K. Rissanen and P. Mal, Mechanochemical Synthesis, Photophysical Properties, and X-ray Structures of N-Heteroacenes. Eur. *J. Org. Chem.*2016, *7*, 1283
4. B. N. Ghosh, F. Topić, P. K. Sahoo, P. Mal, J. Linnera, E. Kalenius, H. M. Tuononen, K. Rissanen, Synthesis, structure and photophysical properties of a highly luminescent terpyridine-diphenylacetylene hybrid fluorophore and its metal complexes. Dalton Trans., 2015, *44*, 254

5. C. Giri*, P. K. Sahoo*, K. Rissanen, P. Mal; Capturing Hydrophobic Trifluoroiodomethane in Water into an M4L6 Cage.*Eur. J. Inorg. Chem.*2016, *31*, 4964 (*contributed equally)

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185. Name : **Ashim Baishya**
Enrolment No. : CHEM11201004012
Date of Award of degree : 23.02.17
Constituent Institute : National Institute of Science Education and Research,
Title : N-Heterocyclic Carbene and its Derivative "Zwitterion" Supported Magnesium and Zinc Complexes: Synthesis, Characterization, Reactivity Studies and Catalytic Applications.

Abstract

N-Heterocyclic carbenes (NHCs) have received much attention in recent years both in main group synthesis and catalysis, due to their strong σ-donating properties.Here, in the present work we have demonstrated the synthesis of NHC supported magnesium andzinc(II) bis(amide) complexes and their catalytic activity towards various organic reactions suchas C–N bond formation reaction of amines with carbodiimides and cross dehydrogenativecoupling of silanes with amines have been studied.Further, a series of NHC stabilized organo-magnesium(II) and -zinc(II) halide complexes are synthesized and structurally characterized. Furthermore, IMes supported organo-magnesium(II)halide complexes are reduced with excess sodium metal in toluene for 3 days to obtain cyclometalatedcompounds of organo-magnesium(II), stabilized by IMes and (*IMes'*) ligands. Theoretical calculations have been carried out on support of the low oxidation state Group 2metal complexes with M–M bond stabilized by NHC.Apart from being used as an excellent neutral ligand system for stabilization of unusual molecules across the periodic table, the strong nucleophilicity of NHC makes its own place as areagent, in synthesizing varieties of organic molecules. Here, we have presented a synthetic wayto zwitterions or "NHC-CDI" adducts. Continuing the synthesis of ligand system, a library of"NHC-CDI" adducts have been synthesized and their coordination behavior with main groupelements, especially with magnesium and zinc has been studied.

Publications

Journal

1. AshimBaishya, V RaoMundlapati, SharanappaNembenna* and Himansu S Biswal*, Structure, bonding and energetics of N-heterocyclic carbene (NHC) stabilized low oxidation state Group 2 (Be, Mg, Ca, Sr and Ba) metal complexes: A theoretical study, *Journal of Chemical Sciences*, 2014, *126*, 6, 1781-1788.
2. AshimBaishya, Milan Kr. Barman, ThotaPeddarao, SharanappaNembenna*, Catalytic C−N bond formation in guanylation reaction by N-heterocyclic carbene supported magnesium(II) and zinc(II) amide complexes, *Journal of Organometallic Chemistry,* 2014,*769*, 112-118.
3. AshimBaishya, ThotaPeddarao, Milan Kr. Barman and SharanappaNembenna*, Catalyst free C–N bond formation by the reaction of amines with diimides: bulky guanidines*, New Journal of Chemistry,* 2015, *39*, 7503-7510,
4. AshimBaishya, Lokesh Kumar, Milan Kr. Barman, ThotaPeddarao andSharanappaNembenna*, Air stable N-heterocyclic carbene-carbodiimide ("NHC-CDI") adducts: bulky amidinates,*ChemistrySelect,* 2016, *3*, 498-503.

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186. Name : **Suvasmita Rath**
Enrolment No. : LIFE11201004016
Date of Award of degree : 23.02.17
Constituent Institute : National Institute of Science Education and Research,
Title : Factors Regulating Epithelial-Mesenchymal Transition and Metastasis of Gastric Cancer.

Abstract

Gastric cancer is ranked as the fourth most common cancer and the second cause of cancer-related mortality in the world. Epithelial to mesenchymal transition (EMT) is the process by which the primary tumor mass leaves its origin and migrates to the distant organs and attains more aggressive metastatic properties. EMT is modulated by hypoxia and *Helicobacter pylori* infection in gastric epithelial cancer cells (GECs). Hypoxia-inducible factor 1α (Hif1α), which is induced by hypoxia as well as *H. pylori* infection, plays a major role in the EMT and metastasis. *H. pylori* infection induces reactive oxygen species (ROS) generation which stabilizes Hif1α in normoxia. *H. pylori* infection also enhances the expression of an antiapoptotic and tumorigenic protein, myeloid cell leukemia 1 (Mcl1), and a proapoptotic and tumor-suppressor protein Noxa. Maintenance of Mcl1 and Noxa balance is a very crucial parameter for cell survival and apoptosis. p300 is a transcriptional cofactor for Hif1α which has histone acetyltransferase (HAT) activity and can function as a tumor-suppressor as well as a proto-oncogene. Most of the metastatic cells are resistant to the existing therapeutic strategies and apoptosis induction in these cells is an absolute requirement to treat metastatic cancers. This thesis work focuses on identifying the molecular mechanism of apoptosis induction in hypoxic and *H. pylori*-infected GECs by modulating p300 HAT and Hif1α activity. This study establishes that HAT inhibition in hypoxic cells induces hydrogen peroxide (H_2O_2)-mediated p38 MAPK activity followed by Noxa upregulation and induction of mitochondria-mediated cell death. HAT inhibition reduces the expression of EMT markers leading to the suppression of metastatic properties in hypoxic GECs. Noxa phosphorylation at S^{13} residue by c-Jun N-terminal kinases (JNKs) induces survival of *H. pylori*-infected GECs by protecting Mcl1 from Noxa-mediated degradation. HAT inhibition results in apoptosis induction selectively in the infected GECs. This work further elaborates on the suppressive effect of p300 HAT inhibition on the EMT, anchorage-independent growth as well as invasiveness of *H. pylori*-infected GECs. Collectively, this work establishes the potential of p300 HAT inhibition on apoptosis induction in hypoxic and *H. pylori*-infected GECs.

Publications

Journal

1. Regulation of Noxa-mediated apoptosis in *Helicobacter pylori*–infected gastric epithelial cells.S Rath, L. Das, S. B. Kokate, B.M. Pratheek, S. Chattopadhyay, C. Goswami,R. Chattopadhyay, S.E. Crowe, A. Bhattacharyya. *FASEB J. 2015 Mar; 29 (3):796-80*6
2. *2 Cobalt chloride-mediated protein kinase Cα (PKCα) phosphorylation induces hypoxia-inducible factor 1α (HIF1α) in the nucleus of gastric cancer cell. $^\#$S. Rath, $^\#$A. Anand, N. Ghosh, L. Das, S. B. Kokate, P. Dixit, S. Majhi, N. Rout, S. P. Singh, A. Bhattacharyya. *Biochem Biophys Res Commun. 2016 Feb 26; 471(1):205-12*
3. *3. Inhibition of histone/lysine acetyltransferase activity kills $CoCl_2$-treated and hypoxia-exposed gastric cancer cells and reduces their invasiveness. S. Rath, L. Das, S. B. Kokate, N. Ghosh, P. Dixit, N. Rout, S. P. Singh, S. Chattopadhyay, H. Ashktorab, D. T. Smoot, M. M. Swamy, T. K. Kundu, S. E. Crowe, A. Bhattacharyya. *International Journal of Biochemistry & Cell Biology volume 82, January 2017, 28-40*
4. ETS2 and Twist1 promote invasiveness of *Helicobacter pylori*-infected gastric cancer cells by inducing Siah2. L. Das, S. B. Kokate, S. Rath, N. Rout, S. P. Singh, S. E. Crowe, A. K. Mukhopadhyay, A. Bhattacharyya. *Biochemical Journal 473 (11), 1629-1640 (2016)*

5. Membrane-bound β-catenin degradation is enhanced by ETS2-mediated Siah1 induction in *Helicobacter pylori*-infectedgastric cancer cells. L. Das, S. B. Kokate, S. Rath, P. Dixit, N. Rout, S.P. Singh, S. E. Crowe, A. Bhattacharyya. *(Communicated-2016)*

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187. Name : **Niru Chowdhury**
Enrolment No. : PHYS11201004013
Date of Award of degree : 23.02.17
Constituent Institute : National Institute of Science Education and Research,
Title : Effect Of Random Anisotropy On Magnetization Reversal In Continuous And Discontinuous Thin Films

Abstract

In this work, magnetization reversal for continuous and discontinuous systems with uniaxial and random anisotropy has been studied. It is shown that in these systems, the presence of random anisotropy along with uniaxial anisotropy affects the reversal, aftereffect relaxation phenomenon and leads to the formation of complicated domain structures.A systematic study on the control of anisotropy has been made by varying the susbtrate rotation during deposition. We found that substrate rotation leads to dispersion in local grain anisotropy and formation of labyrinth domains. Further, we studied the effect of random anisotropy in addition to inter-layer interactions in Co/AlO_x/Co trilayers which leads to layer-by-layer magnetization reversal. We have also shown that random anisotropy is a significant ingredient for the occurrence of 360° domain walls e.g. CoFe/ Al_2O_3 multilayers exhibiting both uniaxial and random anisotropy. The presence of random anisotropy in discontinuous thin films showing superferromagnetic state, results in decrease in ferromagnetic correlation strength and compressed exponential relaxation behaviour.

Publications

Journal

1. "Study of magnetization reversal processes in a thin Co film", N. Chowdhury,S. Bedanta and G. S. Babu, *J. Magn. Magn. Mat.,* 2013, *336*, 20–25.
2. "Effect of inter-particle interactions in magnetic nanoparticle ensembles", S. Bedanta, N. Chowdhury, and W. Kleemann, Sensor Letters, 2013, 11, 1-8.
3. "Controlling the anisotropy and domain structure with oblique deposition and substrate rotation", N. Chowdhury and S. Bedanta, AIP Advances, 2014, 4, 027104-1- 6.
4. "Controlling the size and relaxation dynamics of superferromagnetic domains",N. Chowdhury , S. Bedanta, S. Sing and W. Kleemann,J. Appl. Phys, 2015, 117, 153907-1-5.
5. "Study of magnetization relaxation in Co thin films prepared by substrate rotation",N. Chowdhury, S. Mallick, S. Mallik and S. Bedanta, Thin Solid Films, 2016, 616, 328-334.

188. Name : **Nitin Saurabh**
Enrolment No. : MATH10201005003
Date of Award of degree : 23.02.17
Constituent Institute : Institute of Mathematical Sciences,
Title : Analysis of Algebraic Complexity Classes and Boolean Functions.

Abstract

The thesis is divided into two parts, viz. Algebraic complexity theory and Boolean function analysis.The first part deals with algebraic complexity theory, specifically with algebraic classes. First we study different kinds of reductions and prove lower bounds against them. In particular, we show that sym-Perm is VNP-complete over fields of characteristic other than 2. Then we prove that Cliquep n is not a monotone p-projection of Perm. We also show that multilinear algebraic classes are closed under exponential sums. Next, we define and study polynomial families based on graph homomorphisms.b Using these families we characterise the algebraic classes VBP, VP and VNP. We establish the first instance of natural families of polynomials that are defined independent of the circuit model, and are VP-complete. We further show the utility of homomorphism polynomials by exhibiting explicit polynomial families that are complete for VBP and VNP. Finally, we end the first part with a study of families of polynomials that are of intermediate complexity, that is, in VNP, but neither VNP-hard nor in VP unless PH collapses to the second level. Specifically, we exhibit a list of new natural VNP-intermediate families of polynomials that are defined using basic NP-complete problems. In the second part of this thesis, we study the Fourier Entropy-Influence (FEI) Conjecture, made by Friedgut and Kalai in 1996. We start with establishing upper bounds on Fourier entropy of a Boolean function. These upper bounds are the combinatorial measures associated with a Boolean function that are known to be larger than the influence. These complexity measures include, among others, the logarithm of the number of leaves and the average depth of a parity decision tree. We then show that for the class of Linear Threshold Functions (LTF), the Fourier Entropy is O(p n). It is known that the average sensitivity for the class of LTF is _(p n). We also establish a bound of Od(n1 1 4d+6) for general degree-d polynomial threshold functions. Next we proceed to show that the FEI Conjecture holds for read-once formulas that use AND, OR, XOR, and NOT gates. Finally, we give a general bound involving the first and second moments of sensitivities of a function (average sensitivity being the first moment),which holds for real-valued functions as well.

Publications

Journal

1. Some Complete and Intermediate Polynomials in Algebraic Complexity Theory.Meena Mahajan and Nitin Saurabh. To appear in Theory of Computing Systems –the special issue of CSR 2016.
2. VNP=VP in the multilinear world. Meena Mahajan, Nitin Saurabh, and SébastienTavenas. Information Processing Letters, 2016, 116(2), pp 179-182.
3. Upper Bounds on Fourier Entropy. Sourav Chakraborty, Raghav Kulkarni, SatyanarayanaV. Lokam, and Nitin Saurabh. Theoretical Computer Science, 2016,vol. 654, pp 92-112 – the special issue of COCOON 2015.
4. Homomorphism Polynomials Complete for VP. Arnaud Durand, Meena Mahajan,Guillaume Malod, Nicolas de Rugy-Altherre, and Nitin Saurabh. Chicago Journalof Theoretical Computer Science, 2016, 2016(3).

189. Name : **Narayan Rana**
Enrolment No. : PHYS10201005008
Date of Award of degree : 23.02.17
Constituent Institute : Institute of Mathematical Sciences,
Title : Perturbative QCD corrections to processes at the LHC.

Abstract

This thesis arises in the context of precision measurements at hadron colliders, mainly the Large Hadron Collider (LHC) at CERN. The second phase of LHC has already begun, providing great precisions to many Standard Model (SM) processes, such as Drell-Yan production, production of the Higgs boson and many more. A similar precision from theoretical side also is much needed to distinguish signals from beyond the SM, if any. With this motivation, first we present QCD corrections to Drell-Yan process at third order in threshold limit. We establish the threshold framework and obtain the most precise prediction for this process till date. Next, we present the quark and gluon form factors for the SM energy momentum tensor at three loop. This plays an important role in the perturbative corrections for a generic massive spin-2 production at the LHC. Besides, we find validity of universal infrared structures and principle of leading transcendentality even with spin-2 insertion. We also consider a pseudo-scalar Higgs in supersymmetric models and present third order QCD corrections in the threshold limit. Finally, we compute the decay amplitude of the Higgs boson to a pair of bottom quarks along with a jet considering VFS scheme. This amplitude provides an important contribution also to the production of the Higgs boson along with a jet at second order. We obtain the corresponding matrix elements through proper crossing and analytical continuation.

Publications

Journal

1. “Drell-Yan Production at Threshold to Third Order in QCD”Taushif Ahmed, Maguni Mahakhud, Narayan Rana and V. Ravindran;Phys. Rev. Lett. 113 (2014) 11, 112002
2. “Two-loop QCD corrections to Higgs → b + b + g amplitude”Taushif Ahmed, Maguni Mahakhud, Prakash Mathews, Narayan Rana and V. Ravin-dran; JHEP 1408 (2014) 075
3. “Spin-2 Form Factors at Three Loop in QCD“Taushif Ahmed, Goutam Das, Prakash Mathews, Narayan Rana and V. Ravindran;JHEP 1512 (2015) 084
4. “Pseudo-scalar Higgs Boson Production at Threshold N^3LO and N^3LL QCD” Taushif Ahmed, M.C. Kumar, Prakash Mathews, Narayan Rana and V. Ravindran;Eur. Phys. J. C 76 (2016) 355 [1]

List of other Publications, Not included in the thesis

1. “Two-Loop QCD Correction to massive spin-2 resonance → 3 gluons”Taushif Ahmed, Maguni Mahakhud, Prakash Mathews, Narayan Rana and V. Ravin-dran; JHEP 1405 (2014) 107
2. “Rapidity Distributions in Drell-Yan and Higgs Productions at Threshold to Third Order in QCD”Taushif Ahmed, M. K. Mandal, Narayan Rana and V. Ravindran;Phys. Rev. Lett. 113, 212003 (2014)

190. Name : **Pallab Kanti Dey**
Enrolment No. : MATH08201104005
Date of Award of degree : 23.02.17
Constituent Institute : Harish-Chandra Research Institute
Title : Some Problems In Elliptic Curves And Diophantine Equations.

Abstract

This thesis involves problems related to elliptic curves, Diophantine equations and number sequences. It is divided into five parts of one chapter each.The first chapter is about classifying a family of elliptic curves over rationals which have rank zero over number fields. In fact, this chapter gives the information about a necessary and sufficent condition for elliptic curves over rationals which are having rank zero over number fields.The second chapter is about computing torsion subgroups over number fields for a family of elliptic curves over the rationals. In fact, this chapter computes explicitly torsion subgroups over a class of number fields.The third chapter is about finding an upper bound for the maximal length of an arithmetic progression in coordinates of points on a family of elliptic curves. This chapter deals with the construction of points on a family of elliptic curves over the rationals which are in arithmetic progression.The fourth chapter is about finding out the perfect powers in a product of terms which are coming from certain number sequences like sequnce of balancing numbers and Lucas balancing numbers. Also this chapter gives information about solving a recent conjecture on Diophantine equation using properties of Lucas balancing numbers.The fifth and final chapter is about finding an upper bound for the length of an arithmetic progression which is represented by an integral binary quadratic form whose discriminant is not a perfect square. This chapter also gives information about the representation of three term arithmetic progression by an integral binary quadratic form.

Publications

Journal

1. Length of an arithmetic progression represented by a binary quadratic form, Pallab Kanti Dey and R. Thangadurai, Amer. Math. Monthly, 2014, Vol. 121, no. 10, 932-936.
2. An analogue of Artin's primitive root conjecture, Pallab Kanti Dey and Balesh Kumar, Integers, 2016, Vol. 16, Paper No. A67.
3. Arithmetic progressions on $y^2 = x^3 + k$, Pallab Kanti Dey and Bibekananda Maji, J. Integer Sequence, 2016, Vol. 19, Article 16.7.4.
4. Diophantine equations concerning balancing and Lucas balancing numbers, Pallab Kanti Dey and S. S. Rout, Archiv der Mathematik, 2017, Vol. 108, no. 1, 29-43.
5. Elliptic curves with rank 0 over number fields, Pallab Kanti Dey, Funct. Approx. Comment. Math. 2017, DOI: 10.7169/facm/1585.

191. Name : **Sneh Bala Sinha**
Enrolment No. : MATH08201004005
Date of Award of degree : 24.02.17
Constituent Institute : Institute of Mathematical Sciences,
Title : On The Transcendence Of Certain Numbers And Some Identities.

Abstract

The thesis consists of two themes, Euler's constant and Identities involving multiple zeta values. In the first part, we consider a generalisation of the classical Euler's constant. A special case of these constants was first introduced by Briggs and the notion was later discussed by Lehmer again after which they are known as the Briggs-Lehmer constants. We link these constants to generalized Briggs-Lehmer constants. We discuss the question of transcendence of these generalize numbers. We have shown an identity involving generalised Euler-Briggs constants, Euler's constant and linear forms in logarithms. This generalises as well as gives an alternate proo of an identity of Lehmer. Further, this identity facilitates the investigation of the (conjectural) transcendental nature of generalized Euler-Briggs constants. Investigations of similar type were carried out in a joint work with Gun and Saha in 2014, which involved the interplay between additive and multiplicative characters. This in turn rendered inevitable a careful analysis of multiplicatively independent units in suitable cyclotomic fields. The generalised Lehmer's identity derived here avoids this leading to natural and transparent proofs of the earlier works.It also allows us to prove a stronger result.The importance of these results is to get information about the nature of the Euler's constant that is if we have an element in the set which is algebraic other than the Euler constant then we can explicitly conclude that the Euler's constant is transcendental.In the second part, we generalised identities involving Hurwitz zeta function, multiple zeta values proved by I. Mezo and show that these are transcendental numbers.

Publications

Journal

1. J. Meher and S. B. Sinha, Some infinite sums identities, Czechoslovak Mathematical Journal, volume 65, 819-827, 2015.
2. S. Gun, E. Saha, S. B. Sinha, A Generalization of an identity of Lehmer, Acta Arithmetica, volume 173, 121-131, 2016.

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192. Name : **Piyush Kumar**
Enrolment No. : LIFE09201004022
Date of Award of degree : 09.03.17
Constituent Institute : Tata Memorial Centre
Title : Comparative evaluation of diagnostic efficacy of laser Raman spectroscopy and histopathology in an animal model of oral carcinogenesis.

Abstract

Oral cancers are a major health concern in South Asian nations. Despite advancements in treatment modalities, oral cancers still suffer from a poor 5-year survival rate (~50%), attributable to late detection. Thus, early detection is required for successful management of oral cancers. Currently practiced diagnostic gold-standard, biopsy followed by histopathology, is invasive (and painful), prone to subjective errors and not convenient for repeated sampling. Hence, Raman spectroscopy (RS), a rapid, objective, non-invasive technique, sensitive to tissue biochemistry, could be effective in early diagnosis, as biochemical changes

precede visible morphological alterations during carcinogenesis. RS has shown promising results in diagnosis of several cancers. Such in vivo studies have mostly relied on clinical examination for site of spectral acquisition. Hence, the present study was undertaken on the widely used hamster buccal pouch (HBP) model for RS based investigation of sequential progression of oral carcinogenesis, verified vis-a-vis histopathology. In the first objective, week-wise analysis was carried out using both in vivo and ex vivo approaches. Sensitivity was 70% by week 8, 70 to 80% for week 9 to 11 and 80 to 100% for week 12 to 14. Thus classification increased progressively till 8 weeks, reached a plateau phase between 8 and 12 weeks and finally increased up to 100 % by 14 weeks. In the second objective, spectral models were trained using histopathology and biomarker expression. Results showed increasing incidence of higher pathologies (dysplasia/SCC/G2, G3) with progression of weeks (3% for week 1-3 to 89% for week 12-14). Misclassifications were explored further and it was shown that repeated mechanical irritations may also lead to abnormal changes in tissues. These changes revealed small foci of higher pathologies and also higher expression of cyclin D1, with respect to normal regions. Overall, findings suggest potential of RS in monitoring progression during carcinogenesis in buccal pouch, and in identifying abnormal changes and microheterogenity which may often go unnoticed in clinical examinations and conventional studies wherein tissue extracts/homogenates are employed. Results provide further proof of RS being a potential adjunct for prospective non-invasive, label-free screening in general population, vis a vis conventional screening which is shown to be effective in high risk groups.

Publications

Journal

1. “Raman spectroscopy in experimental oral carcinogenesis: investigation of abnormal changes in control tissues”, P. Kumar, T. Bhattacharjee, M. Pandey, A. Hole, A. Ingle, C. Murali Krishna, Journal of Raman Spectroscopy, 2016.
2. “Raman spectroscopy of experimental oral carcinogenesis: Study on sequential cancer progression in hamster buccal pouch model”, P. Kumar, T. Bhattacharjee, A. Ingle, G.B. Maru, C. Murali Krishna,Technology in Cancer Research and Treatment, 2015.
3. “Animal models in disease diagnosis: Exploration using Raman spectroscopy”, P. Kumar, C. Murali Krishna Asian Journal of Physics, 2015.
4. “Multimodal spectroscopic applications in cancer diagnosis: Combined Raman spectroscopy and Optical coherence tomography”, P. Kumar and C. Murali Krishna, Asian Journal of Physics, 2015.

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193. Name : **Ashwini Kumar**
Enrolment No. : ENGG01201104014
Date of Award of degree : 09.03.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Organic Chemiresistive And Organic Field Effect Transistor Gas Sensors.

Abstract

Flexible gas sensors are a key to futuristic technologies owing to their light weight, low power consumption, integratibility with textile electronics, human body, food wraps and RFID tags etc. Owing to their excellent thermal and chemical stability Cobalt Phthalocyanine (CoPc) and Poly [N-9 heptadecanyl-2, 7-carbazole-alt-5, 5-(4 7 -di-2-thienyl 2 , 1 , 3 benzothiadiazole)] (PCDTBT) have demonstrated their applicability for gas sensors. In the present thesis CoPc and PCDTBT were investigated in details as a sensing layer in chemiresistive and Organic Field Effect Transistor (OFET) sensor configuration, respectively on a flexible biaxially oriented polyethylene terephthalate (BOPET) substrate. In case of Chemiresistive sensor using CoPc, the thickness of the sensing layer has been optimized to be 20 nm. We have achieved remarkably high charge carrier mobility ~ 118 $cm^2V^{-1}s^{-1}$. Such a high charge carrier mobility in CoPc films was attributed to electrostatic interaction of polar groups of BOPET with CoPc molecules and a relatively stronger π-π interaction among CoPc molecules along the molecular chain. These films also exhibited reversible change in resistance on bending to different radii of curvature which suggest their applicability in flexible electronics. These high mobility flexible CoPc films were found to be sensitive to NH_3 in the range 5-50 ppm. In addition, we have demonstrated the significant improvement in sensing properties on application of tensile strain to these flexible CoPc films. Further, in an attempt to make CoPc based chemiresistor more selective towards H_2S gas, these films were modified with a thin layer of gold (~ 1 nm thick). Modification to CoPc film by Au results in the creation of an accumulation layer of hole towards CoPc side which makes these films more reactive for H_2S and were able to sense down to 100 ppb. To improve the response and recovery time of sensor, we have made a heterojunction of CoPc with ZnO Nanowire. It was demonstrated that ZnO Nanowires modified with an optimum thickness of 25 nm of CoPc resulted in H_2S Sensor with better response kinetics. The improvement in response / recovery times is explained on the basis of direct interaction of analyte molecules with oxygen free cobalt sites. Additionally, PCDTBT based OFET sensor was fabricated and characterized and was found to be selective towards NO_2 gas with a minimum detection limit of 1 ppm with a response time of 15 s. Our results suggest that among all ZnO-CoPc (25nm) heterojunction film with a good response percent (275 % at 10 ppm) and fast response kinetics (~13 mins. for 10 ppm) is attractive candidate for practical H_2S sensing applications while PCDTBT based OFET is suitable for NO_2 Sensor.

Publications

Journal

1. "Flexible cobalt-phthalocyanine thin films with high charge carrier mobility", A. Singh, A. Kumar, Ashwini Kumar, S. Samanta, A. K. Debnath, P. Jha, R. Prasad, Z. Salmi, S. Nowak, M. M. Chehimi, D. K. Aswal, S. K.Gupta, *Applied Physics Letters*, 2012, *101*, 222102-5.
2. "Bending stress induced improved chemiresistive gas sensing characteristics of flexible cobalt-phthalocyanine thin films", A. Singh, Ashwini Kumar, A. Kumar, S. Samanta, N. Joshi, V. Balouria, A. K. Debnath, R. Prasad, Z. Salmi, M. M. Chehimi, D. K. Aswal, S. K. Gupta, *Applied Physics Letters,* 2013, *103*, 132107-4.
3. "Room temperature detection of H_2S by flexible gold–cobalt phthalocyanine heterojunction thin films", Ashwini Kumar, N. Joshi, S. Samanta, A. Singh, A. K. Debnath, A. K. Chauhan, M. Roy, R. Prasad, K. Roy, M. M. Chehimi, D. K. Aswal, S. K. Gupta, *Sensors and Actuators B: Chemical*, 2015, *206*, 653-662.
4. "Fast Response and High Sensitivity of ZnO Nanowires - Cobalt Phthalocyanine Heterojunction based H_2S Sensor", Ashwini Kumar, S. Samanta, A. Singh, M. Roy, S. Singh, S. Basu, M. M. Chehimi, K. Roy, N. Ramgir, A. K. Debnath, D. K. Aswal, S. K. Gupta, M. Navneethan, Y. Hayakawa, *ACS Applied Materials & Interfaces*, 2015, *7*, 17713-17724.

194. Name : **Vijay Tailor**
Enrolment No. : LIFE01200904008
Date of Award of degree : 09.03.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Cloning, overexpression and characterization of two peroxiredoxin genes (alr3183 and alr4642) from Anabaena PCC 7120

Abstract

Peroxiredoxins (Prxs) are ubiquitous proteins that detoxify peroxides (such as hydrogen peroxide) using conserved cysteine residues. *Anabaena* PCC 7120 (hereafter referred as *Anabaena*) encodes 10 Prxs, of which two Prxs, Alr3183 and Alr4642, were characterized in this study. Alr3183 showed high similarity to PrxQs from plants (e.g. Arabidopsis). Activity of PrxQs is mediated by two cysteines, peroxidatic (C_p) and resolving (C_r), in association with a reducing partner. Alr3183, which utilized thioredoxin A (TrxA) as reductant for peroxidase activity, was an intramolecular disulfide bond-containing monomeric protein. Alr3183 was an efficient enzyme capable of detoxifying various peroxide substrates. However, Alr3183 lacking C_p (Alr3183C46S) or C_r (Alr3183C51S) formed intermolecular disulphide linkages and was dimeric. Alr3183C46S was completely inactive, while Alr3183C51S required higher concentration of TrxA for peroxidase activity. Surface plasmon resonance analysis showed that unlike Alr3183 or Alr3183C46S, Alr3183C51S bound rather poorly to TrxA, revealing the importance of C_r for interaction with thioredoxins. *In vivo*, Alr3183 was found to be induced in response to γ-radiation. On exposure to H_2O_2, *Anabaena* strain over-expressing Alr3183 showed reduced formation of ROS, intact photosynthetic pigments and consequently better survival than the wild-type, whereas overproduction of Alr3183C46S did not provide any protection. Thus, *in vivo* peroxidase activity of Alr3183 is essential to protect *Anabaena* from the lethal effects of H_2O_2.In *Anabaena,* the ORF *alr4642* encoded a protein that showed homology to Prx-like family of Prxs. Sequence analysis showed the presence of another methionine residue, 35 amino acids away from the first annotated methionine. Similarity of Alr4642 with the other Prx-like proteins was observed only from the second methionine residue. When over-expressed in *E. coli*, both Alr4642 and AlrT4642 (truncated Alr4642, initiating from the second methionine) remained insoluble and could not be purified. Interestingly, expression of the complete *alr4642* ORF in *Anabaena* led to production of the AlrT4642 protein, suggesting that the second ATG was the actual *in vivo* start codon of *alr4642* in *Anabaena*. When over-expressed in *Anabaena*, AlrT4642 (with a C-terminal His-tag) remained soluble and could be purified by affinity chromatography. The purified AlrT4642 protected the plasmid DNA from oxidative damage whereas *Anabaena* cells over-expressing AlrT4642 showed improved resistance to H_2O_2 than the wild-type. These data indicate that AlrT4642 is indeed an antioxidant protein that is capable of defending *Anabaena* from oxidative stress.

Publications

Journal

1. "Over-expression of Alr4642, a novel Prx-like peroxiredoxin, defends the cyanobacterium *Anabaena* PCC7120 from oxidative stress", (2015) Tailor V., Ballal A., Journal of Applied Phycology, 27(6): 2261-2270.
2. "Novel molecular insights into the function and the antioxidative stress response of a Peroxiredoxin Q protein from Cyanobacteria", (2017) Tailor V., Ballal A. Free Radical Biology and Medicine DOI: 10.1016/j.freeradbiomed.2017.01.031.

195. Name : **Sadhana Mukerji**
Enrolment No. : PHYS01200804023
Date of Award of degree : 09.03.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Neutron Induced Cross Section and Fission Yield Measurements for Thorium and Uranium.

Publications

Journal

1. “Measurement of ^{232}Th(n, γ) and ^{232}Th(n, 2n) cross-section at neutron energies of 13.5, 15.5 and 17.28 MeV,” using neutron activation techniques,” Sadhana Mukerji, H. Naik, S. V. Suryanarayana, S. Chachara, B. S. Shivsankar, Sudipta Samanta, B. K. Nayak, A. Saxena, S. C. Sharma, V. Bhagwat, K .K. Rashid, R .N. Jindal, S. Ganesan, A .K. Mohanty, A. Goswami and P. D. Krishnani,Pramana, 79, 249-262 (2012), EXFOR Entry No. 33044.
2. “Application of Neutron Activation Techniques for the Measurement of ^{238}U(n, γ) and ^{238}U(n, 2n) Cross Section at Neutron Energies of 13.5 and 17.28 MeV,” Sadhana Mukerji, H. Naik, S. V. Surayanarayana, B. S. Shivashankar, V. K. Mulik, Sachin Chachara, Sudipta Samanta, A. Goswami and P .D. Krishnani, Journal of Basic and Applied Physics, 2, 104-113 (2013).
2. “Measurements of Fission Product Yield in the neutron-induced fission of ^{238}U with average energies of 9.35 and 12.52 MeV,” Sadhana Mukerji, P. D. Krishnani, B. S. Shivsankar, V. K. Mulik, S .V. Suryanarayana, H. Naik and A. Goswami, Journal of Korean Physical Society, 65, 18-24 (2014).
3. “Measurement of the neutron capture cross-section of ^{238}U at neutron energies of 5.9 ± 0.5 and 15.5 ± 0.7 MeV, by using the neutron activation technique,” V .K. Mulik, S. V. Surayanarayana, H. Naik, Sadhana Mukerji, B. S. Shivsankar, P .M. Prajapati, S .D. Dhole, V. N. Bhoraskar, S. Ganesan and A. Goswami,Annals of Nuclear Energy, 63, 233–240 (2014).
4. “Measurement of fission product yields in the quasi-mono-energetic neutron-induced fission of ^{238}U,” H. Naik, Sadhana Mukerji, Rita Crasta, S.V. Suryanarayana, S.C. Sharma and A. Goswami, Nuclear Phys. A 941 (2015) 16–37.
5. “Measurement of fission products yields in the quasi-mono-energetic neutron-induced fission of ^{232}Th.” H. Naik, Sadhana Mukherji, S.V. Suryanarayana, K.C. Jagadeesan,S.V. Thakare and S.C. Sharma, Nucl. Phys. A 652 (2016) 100-120.

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196. Name : **Sushri Priyadarshini**
Enrolment No. : LIFE11201004006
Date of Award of degree : 09.03.17
Constituent Institute : National Institute of Science Education and Research,
Title : Effects of Psychological Stress on Physiological Homeostasis and Disease Susceptibility.

Abstract

The stress response system has evolved as a survival mechanism that enables organisms to cope with aversive situations. Activation of this system usually puts the body in an energy crisis mode, which if sustained for a prolonged period can adversely affect the body. Psychological stressors are events that are cognitively identified as threat by an organism and can trigger the stress response system. Psychological stress modulates the activity of nervous system, immune system, endocrine system, cardiovascular system,

digestive system, etc. In fact, clinical evidences have linked accumulative allostatic effect of chronic stress induced-dysautonomia to a plethora of organ dysfunction and/or disorders such as chronic-adrenal fatigue, insomnia, high blood pressure, circulation disorders, heart disease, gastrointestinal disorders, obesity, dyslipidemia, diabetes, autoimmune disorders, anxiety disorders, depression, addiction, panic attacks, etc. However, most of these observations are based on physiological parameters and very few studies provide insights to the molecular signaling events. Despite huge upsurge in biomedical reports of psychological stress manifestations in disease outcome, majority of the studies provide observations based on physiological parameters, with very less scattered information on the involved molecular signaling events for understanding the cause and effect relationship of stress and diseases. Due to paucity of integrative analysis, a large amount of relevant information still remains hidden in the unstructured text of published literature. These data, if harnessed for predictive hypothesis generation and targeted experimentation, can cut down on time and resources immensely compared to the traditional methods.To address these issues, the existing technologies in gene-networking have been explored in this thesis, leading to integration of molecular information from scattered studies. The work contributed to this field through development of new methodologies, which could reduce multiple gene centric information in literature to gene-disease and gene-physiology associations and identify new gene-signaling events. In the process, roles of serotonin receptors in adaptive compensatory stress response were predicted. In vitro validation of the predictions established that two predicted serotonin receptors were affected by stress hormones and could induce adipogenesis by peripheral stress hormone signaling within a stress micro-environment in macrophage-adipocyte co-culture systems. Kinetic analysis of genome wide transcriptional profiling of this in-vitro co-culture showed that oxidative metabolism and accumulation of oxidative by-products as the major contributors of inflammation and metabolic dys-regulation that might act as important players in increasing disease susceptibility due to stress. An integrated platform for integration and analysis of psychological stress data generated through systematic gene-networking studies was also developed, and can be used for identifying more gene-signaling events in relation to psychological stress.

Publications

Journal

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2. P. Sood, S. Priyadarshini&P. Aich (2012) Psychological stressors as interventions: Good out of the evil. Front Biosci (Schol Ed), 4: 43-60
3. P. Sood,S. Priyadarshini&P. Aich, (2013) Estimation of Psychological Stress in Humans: A Combination of Theory and Practice. PLoS ONE8, e63044.
4. S. Priyadarshini and P. Aich (2015), A brief overview of stress, stressors and manifestation, Global Meet of Biologists Proceedings, Vol 12(3), 199-212.
5. S. Priyadarshiniand P. Aich. (2016)Understanding effects of Psychological Stress on physiology and disease through human stressome - An integral algorithm. Current Bioinformatics, 11(2), 277-290
6. S. Priyadarshini, B. Pradhan& P. Aich. Cortisol mediated regulation of immune and metabolic processes in murine adipocytes 3T3-L1 and macrophages RAW 264.7 via serotonin receptors HTR2a and HTR5c (Communicated)
7. S. Priyadarshini, B. Pradhan& P. Aich. Effects of Cortisol and Serotonin onPre-adipocytes and Macrophages of Mouse Origin: A Shift in Immune Response kinetics (communicated)

197. Name : **Ashutosh Kumar**
Enrolment No. : LIFE11201004001
Date of Award of degree : 09.03.17
Constituent Institute : National Institute of Science Education and Research,
Title : Importance of TRPV4 channel in the mitochondrial structure-function relationship: Implication in pain and other pathophysiology.

Abstract

TRPV4 is a non-selective cation channel belong to TRP super family of ion channels and can be activated by different physical stimuli such as by physiological temperature, osmolarity, electromagnetic waves, mechanical stretch as well as by chemicalstimuli such as different endogenous ligands and lipid derivatives. At the cellular level, TRPV4 regulates complex signalling eventsand maintain intracellular Ca^{2+}-levels. So far a large number of studies indicate that TRPV4is involved in sensory functions and abnormalities in its regulation and functionsaffect diverse type of cells and tissues resulting in the development of several pathophysiological conditions. Indeed, point-mutations in this channel also correlate well with the development of inheritable syndromes such as CMT, SMDand different forms of neuropathic pains. However, the molecular mechanisms behind such pathophysiologies are not well understood.This thesis work explored TRPV4 in the context of mitochondrial localization and functions. EndogenousTRPV4 is not only present in the mitochondria but also regulates its critical functions in neuronal and non-neuronal systemssuch as in neurons and in mature sperms.TRPV4 has a unique Mitochondrial Targeting Signal (MTS) which is highly conserved throughout vertebrate evolution. TRPV4 interacts with key mitochondrial proteins namelywith Mfn1, Mfn2, Hsp60 and also with Cyt-C. TRPV4 activation regulates mitochondrial morphology, fission and fusion, oxidative potential, Ca^{2+}-influx,energeticsand metabolism;both *in vivo* and *in vitro* conditions. Among all, physical interaction of TRPV4 with metabolites involved in sterol and steroid bio-synthesis pathway ishighly relevant for several physiological as well as pathophysiological conditions. Regulation of mitochondrial morphology, functionsand metabolism by TRPV4 has broad implications in the molecular understandings of certain mitochondria-specific functions and mechanisms in details.

Publications

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2. Kumar A, Goswami L, Goswami C (2013) Importance of TRP channels in pain: implications for stress. *Frontiers in Bioscience*. (*Schol Ed*) 5, 19-38
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4. ‡*Majhi RK, *Kumar A, Yadav M, Swain N, Kumari S, Saha A, Pradhan A, Goswami L, Saha S, Samanta L, Maity A, Nayak TK, Chattopadhyay S, Rajakuberan C, Kumar A, Goswami C. (2013) Thermosensitive ion channel TRPV1 is endogenously expressed in the sperm of a fresh water teleost fish (*Labeorohita*) and regulates sperm motility. *Channels*7, 1-10
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6. *Kumari S, *Kumar A, *Sardar P, Yadav M, Majhi RK, Kumar A, Goswami C. (2015) Influence of membrane cholesterol in the molecular evolution and functional regulation of TRPV4.*BiochemBiophys Res Commun.*456, 312-9
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8. Kumar A, Majhi RK, Swain N, Giri SC, Kar S, Samanta L, Goswami C. (2016) TRPV4 is endogenously expressed in vertebrate spermatozoa and regulates intracellular calcium in human sperm. *BiochemBiophys Res Commun.*473 (4):781-8.

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198. Name : **Susmita Dhara**
Enrolment No. : PHYS05201004005
Date of Award of degree : 09.03.17
Constituent Institute : Saha Institute of Nuclear Physics,,
Title : Preparation, Characterization and Study of Magnetic Properties of $Co_{X} Cu_{1-X}$ (0.01≤x≤ 0.7) Granular Alloys.

Abstract

Co_xCu_{1-x} (x ~ 0.01-0.76) nanosized particles were prepared by chemical reduction of $CoCl_2$ and $CuCl_2$ in solution with CTAB being used for capping of the alloy particles. Average cobalt content (x) in these alloys were obtained from inductively coupled plasma optical emission spectroscopic (ICPOES) measurements. Transmission electron microscopy (TEM) results showed particles of mean size ~ 15 nm existing in lumps and filament-like formations. The measured lattice spacings from selected area diffraction (SAD) pattern confirms that the alloy is formed in *fcc* crystalline phase as in copper. Lowest Co-content ~ 0.01 mol % sample shows identical paramagnetic behavior in both ZFC and FC magnetization measurements. For other samples, there is a peak in ZFC magnetization at a certain temperature and ZFC/FC magnetization bifurcate at a higher temperature, which for high Co containing samples is close to room temperature. Samples are characterized by blocking temperature (T_B) distributions of SPM clusters resulting from variations in particle size and inhomogeneities in their chemical compositions. Such variations are reflected also in data obtained from TRM studies. All the samples except Co-0.01 exhibit hysteresis loops at 4-300 K. Analysis shows that FM contribution increases and SPM contribution decreases with increase in Co content. At low Co concentration the sample is entirely superparamagnetic but at high Co concentration the sample magnetization is a combination of superparamagnetism and ferromagnetism. It is clear from the above results that in samples ~ 0.01-0.33 mol %, there is a FM part growing in size with Co content, together with a SPM part. As the samples have almost the same average saturation magnetic moment per Co atom independent of Co concentration, there is a possibility of occurrence of a Co rich core and Cu rich shell type structure. A significant temperature dependent exchange bias field is obtained from above 100 K down to 2 K suggest that the particles have a Co rich SPM core, surrounded by uncompensated dilute Co spin moments at the surface. Also, the sample exhibits a weak spin-glass like ordering occurring at ~7 K. The overall behavior of the system is that of an assembly of almost non-interacting magnetic nanoparticles as suggested by the study of relaxation of magnetization. If during relaxation certain external conditions are temporarily disturbed, e.g., by lowering the temperature or changing the magnetic field the magnetization also changes accordingly; but as the conditions are restored the magnetization returns to its previous value. Such magnetic 'memory effect' has been studied with various experimental protocols and persists strongly even at room temperature. Lastly, in temperature dependence in electrical resistivity, samples with low cobalt content of x ≤ 0.1 show a metallic resistivity behavior. For samples with higher cobalt content, x ≥ 0.17, the resistivity shows a minimum. The minimum becomes more pronounced as Co content (x) increases and also the temperature of minimum resistivity, T_{min}, increases with x. Such trends continue even when x is as high as ~ 76 %. Application of an external magnetic field has negligible effect on the resistivity behavior. Detailed analysis suggests that the low temperature upturn in resistivity most probably arises due to elastic electron-electron interaction (quantum interference effect). Combining the results of the two types of measurements, a model of formation of these alloy particles involving random clusters of Co atoms within Cu matrix has been proposed.

Publications

Journal

1. Synthesis, characterization and magnetic properties of CoxCu$_{1-}$x(x∼0.01–0.3) granular alloys, S. Dhara, R. Roy Chowdhury, S. Lahiri, P. Ray, B. Bandyopadhyay' Journal of Magnetism and Magnetic Materials , 374, 647–654 (2014).
2. Strong memory effect at room temperature in nanostructured granular alloy Co$_{0.3}$Cu$_{0.7}$,S Dhara, R. Roy Chowdhury, B. Bandyopadhyay, RSC Advances, 5, 95695 (2015).
3. Observation of resistivity minimum in low temperature in nanostructured granular alloys CoxCu1-x (x<.17-0.76), S. Dhara, R. Roy Chowdhury, B. Bandyopadhyay, Phys, Rev. B, 93, 214423, ()2016.

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199. Name : **Surbhi Jaiswal**
Enrolment No. : PHYS06201204001
Date of Award of degree : 21.03.17
Constituent Institute : Institute For Plasma Research,
Title : Nonlinear Excitations In Flowing Complex Plasmas.

Abstract

Equilibrium plasma flows occur in many natural situations such as in galactic jets, solar wind etc. as well as in magnetic and inertial fusion experiments. The encounter of such plasma flows with a stationary charged object can give rise to a rich variety of dynamical phenomena such as one observes in the interaction of the solar wind with the earth or other planets. The study of such an interaction in a laboratory setting can provide much insight into fundamental processes governing linear and nonlinear collective excitations arising from the encounter. Adusty plasma, consisting of micron or submicron sized particles immersed in an electron-ionplasma, provides a unique platform and a convenient tool to explore such phenomena. The highly massive bigger sized particles gets negatively charged due to collection of more electrons than ions and constitute a cloud which can be identified by illuminating through laser and their dynamics can be captured by normal CCD camera. Thus it provides various diagnostic conveniences over two component plasma and hence an excellent medium to study flow induced phenomena. In this thesis we have carried out experimental and theoretical investigation of different nonlinear waves and structures in flowing complex plasma. Primary focus is to investigate the various techniques of flow generation, fast moving precursor soliton excitation in the upstream region along with the wake in the downstream region of flowing dust generated by means of altering potential hill and the neutral gas induced shock wave excitation in dusty plasma. The experiments have been carried out in a newly built ∏ - shaped Dusty Plasma Experimental (DPEx) device. The device has been fabricated and installed in the Institute for Plasma Research which has several inbuilt facilities for flowing plasma studies. The experiments have been performed in the DC glow discharge plasma generated between disc shaped anode and long grounded cathode tray in the background of Ar gas. A detailed characterization of plasma and dusty plasma has been done by using various electric probes and standard techniques of image analysis. Three different techniques of flow generation based on neutral streaming and altering potential hill have been explored and different tools to measure the flow velocity including a novel technique of dust acoustic wave excitation are used in the experiments. A phenomenon of precursor soliton is observed for the first time in the charge medium by flowing the dust fluid over a biased potential hill. A theoretical explanation of these excitations based on the forced Korteweg-de Vries model equation is provided and their practical implications in situation involving a charged object moving in plasma are discussed. A flow induced dispersive dust acoustic shock wave has been observed when flow velocity exceeded the Mach number 2. The observed evolution of the shock waves and

their propagation characteristics are found to compare well with model numerical results based on a modified Korteweg-de- Vries- Burgers type equation.

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2. “Experimental investigation of flow induced dust acoustic shock waves in a complexplasma”, S. Jaiswal, P. Bandyopadhyay and A. Sen, Physics of Plasmas, 2016, 23, 083701.
3. “Experimental observation of precursor solitons in a flowing complex plasma”,S.Jaiswal, P. Bandyopadhyay and A.Sen, Physical Review E, 2016, 93, 041201(R).
4. “Dusty Plasma Experimental (DPEx) device for complex plasma experiments withflow”, S. Jaiswal, P. Bandyopadhyay and A.Sen, Review of Scientific Instruments,2015, 86, 113503.
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6. “Vortex shedding in flow past an obstacle”, S. Jaiswal, P. Bandyopadhyay and A.Sen, (Under Preparation), 2016

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200. Name : **Prabhat Kumar Sahu**
Enrolment No. : CHEM11201104004
Date of Award of degree : 22.03.17
Constituent Institute : National Institute of Science Education and Research,
Title : Towards Understanding Solute and Solvent Dynamics in Mono and Dicationic Room Temperature Ionic Liquids Through Fluorescence and Nuclear Magnetic Resonance (NMR) Studies

Abstract

In recent times, room temperature ionic liquids (RTILs) have attracted considerable attention both from academia and industry mainly due to their attractive physicochemical properties and their use in several applications. Geminaldicationic ionic liquids (DILs), having two unit positive charge, are expected to be advantageous over traditional monocationic ionic liquids (MILs) as DILs have been shown to possess superior physicochemical properties in contrast to MILs. In this regard, studies that focus in understanding the structure-dynamics correlation in these special media are of extreme importance for effective utilization of these systems. The main objective of the present thesis is to understand the structure-dynamics correlation through solute rotation and solvation dynamics study in both MILs and DILs. A brief introduction on RTILs and basic principles of solute and solvent dynamics phenomena are discussed in the first chapter of the thesis. The instrumentation techniques and methodologies adopted for data analysis are discussed in the second chapter. The third and fourth chapter discuss the effect of ion-ion interaction on rotational dynamics and effect of solvation dynamics on intramolecularphotoinduced electron transfer process in fluorescent molecules respectively. Effect of cosolvents on solute-solvent and solvent-solvent interactions in a borate-based RTIL is discussed in the fifth chapter. A comparative study on solute and solvent relaxation dynamics in imidazolium-based MILs and a DIL through a combined fluorescence and NMR investigations is presented in the sixth chapter. Summary and future prospects are also outlined at the end of the last chapter.

Publications

Journal

1. Photophysical and density functional studies on the interaction of a new nitrobenzoxadiazole derivative with anions. S. K. Das, S. S. Mishra; P. K. Sahu, A. Nijamudheen, V. Mohan,; M. Sarkar. *Chem. Phys. Lett.* 2012*, 528*, 11.
2. Ion interactions with a new ditopicnaphthalimide-based receptor: A photophysical, NMR and theoretical (DFT) Study. V. Mohan, A. Nijamudheen, S. K. Das,P. K. Sahu, U. P. Kar, A. Rahaman, M. Sarkar. *ChemPhysChem*2012, *13*, 3882.
3. *Picosecond solvation dynamics of Coumarin153 in Bis(1-Methyl-1h-Imidazol-3-Ium-3-Yl)dihydroborate cation containing room temperature ionic liquid and ionic liquid-dmf mixtures.P. K. Sahu, S. K. Das, M. Sarkar. *J. Appl. Sol. Chem. Model.*, 2013, *2*, 47.
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5. Probing the microscopic aspects of 1-butyl-3-methylimidazolium trifluoroacetate ionic liquid and its mixture with water and methanol: A photophysical and theoretical (DFT) study. S. K. Das, P. K. Sahu, M. Sarkar. *J. Fluoresc.* 2013, *23*, 1217.
6. Diffusion−viscosity decoupling in solute rotation and solvent relaxation of coumarin153 in ionic liquids Containingfluoroalkylphosphate (FAP) Anion: A thermophysical and photophysical study. S. K. Das, P. K. Sahu, M. Sarkar. *J. Phys. Chem. B* 2013*, 117*, 634.
7. *Toward understanding solute−solvent interaction in room-temperature mono- and dicationic ionic liquids: A combined fluorescence spectroscopy and mass spectrometry analysis.P. K. Sahu, S. K. Das, M. Sarkar. *J. Phys. Chem. B*2014, *118*, 1907.
8. *Fluorescence response of a dipolar organic solute in a dicationic ionic liquid (IL): Is the behavior of dicationic IL different from that of usual monocationic IL? P. K. Sahu, S. K. Das, M. Sarkar. *Phys. Chem. Chem. Phys.*2014, *16*, 12918.
9. Probing the aggregation behavior of 4-aminophthalimide and 4-(N,N-dimethyl) amino-N-methylphthalimide: a combined photophysical, crystallographic, microscopic and theoretical (DFT) study. D. Majhi, S.K. Das, P. K. Sahu, S. Md Pratik, A. Kumar , M. Sarkar.*Phys. Chem. Chem. Phys.,* 2014, *16*, 18349.
10. Analyte Interactions with a new ditopicdansylamide−nitrobenzoxadiazole dyad: a combined photophysical, NMR, and theoretical (DFT) study. A. K. Bhoi, S. K. Das, D.Majhi, P. K. Sahu, A. Nijamudheen, N. Anoop, A. Rahaman, M. Sarkar. *J. Phys. Chem. B*2014, *118*, 9926.
11. Studies on electronic energy transfer (EET) on a series of room temperature ionic liquids (RTILs):can the EET studies on RTILs be exploited to predict their structural organization? S. K. Das, P. K. Sahu, M. Sarkar.*RSC Adv.,*2014, *4*, 39184.
12. *Understanding structure-property correlation in monocationic and dicationic ionic liquids through combined fluorescence and pulsed-field gradient (PFG) and relaxation NMR experiments.P. K. Sahu, A. Ghosh, M. Sarkar. *J. Phys. Chem. B*, 2015,*119*, 14221.
13. Investigating the influence of alkyl side chain length on the fluorescence response of C153 in a series of room temperature ionic liquids. S. K. Das, D. Majhi, P. K. Sahu, M. Sarkar. *RSC Adv.,*2015, *5*, 41585.
14. Combined photophysical, NMR and theoretical (DFT) study on the interaction of a multi component system in absence and presence of different biologically and environmentally important ions. A. K. Bhoi, P. K. Sahu, G. Jha. M. Sarkar.*RSC Adv*., 2015, *5*, 61258.

15. *Studies on intramolecular electron transfer reaction in donor-spacer-acceptor systems in room-temperature ionic liquids.P. K. Sahu, S. K. Das, M. Sarkar.*J. Mol. Liq.*2016, *214*, 24.
16. *Reorientational dynamics of charged and neutral solutes in 1-Alkyl-3-methylimidazoilum Bis(trifluoromethylsulfonyl)imide ionic liquids: Realization of ionic component of hydrogen bond.P. K. Sahu, M. Sarkar.*Chem. Phys.Lett.,* 2016, 652, 177.
17. Studies on the mechanism of fluorescence quenching of cds quantum dots by 2-amino-7-nitrofluorene and 2-(n,n-dimethylamino)-7-Nitrofluorene. S. S. Dandpat, P. K. Sahu, M. Sarkar. *Chemistry Select*, 2016,*1*, 2219.
18. Probing interactions of structurally similar but chemically distinguishable organic solutes with 1-ethyl-3-methylimidazolium alkylsulfate(alkyl = ethyl, hexyl and octyl) ionic liquids through fluorescence, NMR and Fluorescence Correlation Spectroscopy (FCS) study. D. Majhi, P. K. Sahu, S. Seth, M. Sarkar, *Phys. Chem. Chem. Phys.*2016, *18*, 22343.
19. *Nuclear magnetic resonance, fluorescence correlation spectroscopy and time-resolved fluorescence anisotropy studies of intermolecular interactions in Bis(1-methyl-1h-imidazol-3-ium-3-yl)dihydroboratebis(trifluoromethylsulfonyl)amide and its mixtures with various cosolvents. P. K. Sahu, R. Nanda, S. Seth, A. Ghosh, M. Sarkar. *Chem. Phys. Lett.*, 2016, *661*, 100.

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201. Name : **Prabhat Kumar Sahu**
Enrolment No. : CHEM11201104004
Date of Award of degree : 22.03.17
Constituent Institute : National Institute of Science Education and Research,
Title : Towards Understanding Solute and Solvent Dynamics in Mono and Dicationic Room Temperature Ionic Liquids Through Fluorescence and Nuclear Magnetic Resonance (NMR) Studies

Abstract

In recent times, room temperature ionic liquids (RTILs) have attracted considerable attention both from academia and industry mainly due to their attractive physicochemical properties and their use in several applications. Geminaldicationic ionic liquids (DILs), having two unit positive charge, are expected to be advantageous over traditional monocationic ionic liquids (MILs) as DILs have been shown to possess superior physicochemical properties in contrast to MILs. In this regard, studies that focus in understanding the structure-dynamics correlation in these special media are of extreme importance for effective utilization of these systems. The main objective of the present thesis is to understand the structure-dynamics correlation through solute rotation and solvation dynamics study in both MILs and DILs. A brief introduction on RTILs and basic principles of solute and solvent dynamics phenomena are discussed in the first chapter of the thesis. The instrumentation techniques and methodologies adopted for data analysis are discussed in the second chapter. The third and fourth chapter discuss the effect of ion-ion interaction on rotational dynamics and effect of solvation dynamics on intramolecularphotoinduced electron transfer process in fluorescent molecules respectively. Effect of cosolvents on solute-solvent and solvent-solvent interactions in a borate-based RTIL is discussed in the fifth chapter. A comparative study on solute and solvent relaxation dynamics in imidazolium-based MILs and a DIL through a combined fluorescence and NMR investigations is presented in the sixth chapter. Summary and future prospects are also outlined at the end of the last chapter.

Publications

Journal

1. Photophysical and density functional studies on the interaction of a new nitrobenzoxadiazole derivative with anions. S. K. Das, S. S. Mishra; P. K. Sahu, A. Nijamudheen, V. Mohan,; M. Sarkar. *Chem. Phys. Lett.* 2012*, 528*, 11.
2. Ion interactions with a new ditopicnaphthalimide-based receptor: A photophysical, NMR and theoretical (DFT) Study. V. Mohan, A. Nijamudheen, S. K. Das,P. K. Sahu, U. P. Kar, A. Rahaman, M. Sarkar. *ChemPhysChem*2012, *13*, 3882.
3. *Picosecond solvation dynamics of Coumarin153 in Bis(1-Methyl-1h-Imidazol-3-Ium-3-Yl)dihydroborate cation containing room temperature ionic liquid and ionic liquid-dmf mixtures.P. K. Sahu, S. K. Das, M. Sarkar. *J. Appl. Sol. Chem. Model.*, 2013, *2*, 47.
4. Synthesis, photophysics, live Cell imaging and aggregation behaviour of some structurally similar alkyl chain containing bromonaphthalimide systems: influence of alkyl chain length on the aggregation behaviour. M. Soni, S. K. Das,P. K. Sahu, U. P. Kar, A. Rahaman, M. Sarkar. *J. Phys. Chem. C* 2013, *117*, 14338.
5. Probing the microscopic aspects of 1-butyl-3-methylimidazolium trifluoroacetate ionic liquid and its mixture with water and methanol: A photophysical and theoretical (DFT) study. S. K. Das, P. K. Sahu, M. Sarkar. *J. Fluoresc.* 2013, *23*, 1217.
6. Diffusion−viscosity decoupling in solute rotation and solvent relaxation of coumarin153 in ionic liquids Containingfluoroalkylphosphate (FAP) Anion: A thermophysical and photophysical study. S. K. Das, P. K. Sahu, M. Sarkar. *J. Phys. Chem. B* 2013*, 117*, 634.
7. *Toward understanding solute−solvent interaction in room-temperature mono- and dicationic ionic liquids: A combined fluorescence spectroscopy and mass spectrometry analysis.P. K. Sahu, S. K. Das, M. Sarkar. *J. Phys. Chem. B*2014, *118*, 1907.
8. *Fluorescence response of a dipolar organic solute in a dicationic ionic liquid (IL): Is the behavior of dicationic IL different from that of usual monocationic IL? P. K. Sahu, S. K. Das, M. Sarkar. *Phys. Chem. Chem. Phys.*2014, *16*, 12918.
9. Probing the aggregation behavior of 4-aminophthalimide and 4-(N,N-dimethyl) amino-N-methylphthalimide: a combined photophysical, crystallographic, microscopic and theoretical (DFT) study. D. Majhi, S.K. Das, P. K. Sahu, S. Md Pratik, A. Kumar , M. Sarkar.*Phys. Chem. Chem. Phys.,* 2014, *16*, 18349.
10. Analyte Interactions with a new ditopicdansylamide−nitrobenzoxadiazole dyad: a combined photophysical, NMR, and theoretical (DFT) study. A. K. Bhoi, S. K. Das, D.Majhi, P. K. Sahu, A. Nijamudheen, N. Anoop, A. Rahaman, M. Sarkar. *J. Phys. Chem. B*2014, *118*, 9926.
11. Studies on electronic energy transfer (EET) on a series of room temperature ionic liquids (RTILs):can the EET studies on RTILs be exploited to predict their structural organization? S. K. Das, P. K. Sahu, M. Sarkar.*RSC Adv.,*2014, *4*, 39184.
12. *Understanding structure-property correlation in monocationic and dicationic ionic liquids through combined fluorescence and pulsed-field gradient (PFG) and relaxation NMR experiments.P. K. Sahu, A. Ghosh, M. Sarkar. *J. Phys. Chem. B*, 2015,*119*, 14221.
13. Investigating the influence of alkyl side chain length on the fluorescence response of C153 in a series of room temperature ionic liquids. S. K. Das, D. Majhi, P. K. Sahu, M. Sarkar. *RSC Adv.,*2015, *5*, 41585.
14. Combined photophysical, NMR and theoretical (DFT) study on the interaction of a multi component system in absence and presence of different biologically and environmentally important ions. A. K. Bhoi, P. K. Sahu, G. Jha. M. Sarkar.*RSC Adv*., 2015, *5*, 61258.

15. *Studies on intramolecular electron transfer reaction in donor-spacer-acceptor systems in room-temperature ionic liquids.P. K. Sahu, S. K. Das, M. Sarkar.*J. Mol. Liq.*2016, *214*, 24.
16. *Reorientational dynamics of charged and neutral solutes in 1-Alkyl-3-methylimidazoilum Bis(trifluoromethylsulfonyl)imide ionic liquids: Realization of ionic component of hydrogen bond.P. K. Sahu, M. Sarkar.*Chem. Phys.Lett.,* 2016, 652, 177.
17. Studies on the mechanism of fluorescence quenching of cds quantum dots by 2-amino-7-nitrofluorene and 2-(n,n-dimethylamino)-7-Nitrofluorene. S. S. Dandpat, P. K. Sahu, M. Sarkar. *Chemistry Select*, 2016,*1*, 2219.
18. Probing interactions of structurally similar but chemically distinguishable organic solutes with 1-ethyl-3-methylimidazolium alkylsulfate(alkyl = ethyl, hexyl and octyl) ionic liquids through fluorescence, NMR and Fluorescence Correlation Spectroscopy (FCS) study. D. Majhi, P. K. Sahu, S. Seth, M. Sarkar, *Phys. Chem. Chem. Phys.*2016, *18*, 22343.
19. *Nuclear magnetic resonance, fluorescence correlation spectroscopy and time-resolved fluorescence anisotropy studies of intermolecular interactions in Bis(1-methyl-1h-imidazol-3-ium-3-yl)dihydroboratebis(trifluoromethylsulfonyl)amide and its mixtures with various cosolvents. P. K. Sahu, R. Nanda, S. Seth, A. Ghosh, M. Sarkar. *Chem. Phys. Lett.*, 2016, *661*, 100.

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202. Name : **Papiya Ghosh**
Enrolment No. : CHEM01201104005
Date of Award of degree : 22.03.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Asymmetric Synthesis Of Some Biologically Relevant Oxygenated Heterocyclic Compounds

Publications

Journal

1. Ghosh, P.; Chattopadhyay, A. A practical procedure of propargylation ofaldehydes. *Tetrahedron Lett*. **2012**, *53*, 5202–5205. (published)
2. Ghosh, P.; Gamre, S. S.; Chatterjee, S.; Chattopadhyay, S.; Sharma, A. AnEnantioselective Synthesis of Clonostachydiol. *Asian J. Org. Chem*. (underrevision)

Conferences

1. P. Dey, S. Gamre, A. Sharma, S. Chattopadhyay. Asymmetric synthesis ofClonostachydiol –a DOS mediated approach, National Conference on Chirality-2015
2. P. Dey, B. B. Dhotare, K. S. Ajish Kumar, A. Sharma. A Practical AsymmetricSynthesis of the Tumor –imaging Agent, 18F-FLT, 6th International Symposiumon Current Trends in Drug Discovery and Research (CTDDR)-2016Papiya Ghosh

203. Name : **Subhasis Pati**
Enrolment No. : CHEM01201204021
Date of Award of degree : 22.03.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : Palladium Based Dense Metallic Membranes for Purification of Hydrogen Isotopes.

Abstract

The purification of hydrogen isotopes attracted considerable interest in the last few decades because of increasing demand of ultrapure gases for fuel cell and fusion reactor applications. Classically, palladium membrane is in use for the purification of hydrogen isotopes to produce ultrapure gases due to high temperature compatibility and high hydrogen flux. However, surface poisoning of pure Pd membrane decreases the hydrogen flux whereas hydrogen embrittlement results in membrane cracking. Similarly, high cost of pure Pd limits its use in commercial scale. Hence, there is a need to overcome these issues for industrial application of Pd membranes for hydrogen purification. Alloying Pd with suitable elements such as Ag, Cu, Au etc. in required proportion is thought to overcome these issues. This thesis work is aimed at developing Pd-based dense metallic membranes for purification of hydrogen isotopes. The preparation of Pd alloy membranes by conventional metallurgical route and supported membranes through electroless plating method were employed in this study. The membranes were characterized by using different techniques such as XRD, TXRF, SEM and EDS. Thermal expansion of these alloys were measured by using high-temperature X-ray diffraction technique. Membrane module with an ultra-high vacuum gas manifold was fabricated and hydrogen permeation experiments were carried out to derive permeation parameters. The H2 and D2 flux were measured at different temperatures and trans-membrane pressures. Thermodynamics and kinetics of hydrogen and deuterium sorption studies on these alloys were investigated. The thesis work results in development of a suitable Pd-Ag-Cu alloy membrane having higher hydrogen flux than the conventional Pd metal membrane. This thesis is divided into four chapters as outlined below.

Publications

Journal

1. Pd-Ag-Cu dense metallic membrane for hydrogen isotope purification and recovery at low pressures. Subhasis Pati, R A. Jat,, N. S. Anand, D. J. Derose, K.N. Karn, S.K. Mukerjee, S.C. Parida, J. Memb. Sci. 522 (2017) 151-158.
2. (2) X-ray diffraction study of thermal parameters of Pd, Pd-Ag and Pd-Ag-Cu alloys as hydrogen purification membrane materials. Subhasis Pati, R. A. Jat, S.C. Parida, S. K. Mukerjee. Physica B. 484 (2016) 42-47.
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4. Thermodynamics and kinetics of hydrogen/deuterium absorption–desorption in Pd0.77Ag0.23 alloy. N. S Anand, Subhasis Pati, R. A. Jat, S. C. Parida and S. K. Mukerjee. Int. J. Hydrogen Energy. 40 (2015) 444-450.

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i. Hydrogen/Deuterium absorption kinetic studies on Pd0.77Ag0.23 alloy. Subhasis Pati, N. S. Anand, Ram Avatar Jat, S. C. Parida, S. K. Mukerjee. DAE-BRNS 5th Interdisciplinary Symposium on Material Chemistry (ISMC-2014), Dec 9-13, 2014, Mumbai, pp-321.

ii. Pressure-Composition- Temperature studies on Pd0.77Ag0.23 –H2/D2 Systems. N. S Anand, Subhasis Pati, R. A. Jat, S. C. Parida, S. K. Mukerjee. DAE-BRNS 5th Interdisciplinary Symposium on Material Chemistry (ISMC-2014), Dec 9-13, 2014, Mumbai, pp-319.

iii. Thermal expansion studies of Pd0.77Ag0.23 alloy using high temperature X-ray diffraction technique. Subhasis Pati, Ram Avtar Jat , S.C. Parida, S. K. Mukerjee. DAE, BRNS Symposium and Workshop on Thermal Analysis (THERMANS-2016), pp-57.

iv. Pressure-Composition-Temperature studies on Pd0.90Cu0.10 –H2/D2 Systems. N. S Anand, Subhasis Pati, R. A. Jat, S. G. Sawant, S. C. Parida, S. K. Mukerjee. DAE, BRNS, Symposium and Workshop on Thermal Analysis (THERMANS- 2016), pp-56.

v. Synthesis and characterization of Pd-Ag alloy by electroless plating method. Subhasis Pati, R. A Jat, S. C. Parida. DAE-BRNS 6th Interdisciplinary Symposium on Material Chemistry (ISMC-2016), Dec 6-10, 2016, Mumbai, pp- 194.

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204. Name : **Priyanka Ganpat Bhosale**
Enrolment No. : LIFE09200904017
Date of Award of degree : 22.03.17
Constituent Institute : Tata Memorial Centre
Title : Genomic Profiling Of Oral Precancerrous Lesions And Early Stages Of Oral Cancer.

Abstract

We present an integrative genome-wide analysis of copy number alterations (CNAs) and gene expression changes in HPV negative, gingivobuccal complex (GBC) pre-cancerous lesions (leukoplakia) and oral squamous cell carcinoma (OSCC) patients. We could identify CNAs and differentially expressed transcripts that can be used to predict the risk of progression from leukoplakia to OSCC. The genomic profiles of leukoplakia resemble those observed in the later stages of OSCC and that several changes are associated with this progression, including amplification of 8q24.3, deletion of 8p23.2, and dysregulation of *DERL3, EIF5A2, ECT2, HOXC9, HOXC13, KRT76, MAL, MFAP5* and *NELL2*. Furthermore, for the first time we demonstrated that *KRT76* loss is one of the early event, but not essential for cell transformation. Comparing copy number profiles of primary tumors with and without lymph node metastasis, we identify alterations associated with nodal metastasis, including amplifications of 3p26.3, 8q24.21, 11q22.1 and 11q22.3 and deletion of 8p23.2. Additional analysis demonstrated up regulation of *BIRC2*(cIAP1) and *BIRC3*(cIAP2) in tumor samples with lymph node metastasis and based on functional validation we could identify role of cIAP2 (*BIRC3*) in lymph node metastasis in SCC29B cells. Integrative analysis reveals several biomarkers that have never or rarely been reported in previous OSCC studies, including amplifications of 1p36.33 (attributable to *MXRA8*), 3q26.31 (*EIF5A2*), 9p24.1 (*CD274*), and 12q13.2 (*HOXC9* and *HOXC13*). Additionally,

we find that amplifications of 1p36.33 and 11q22.1 are strongly correlated with poor clinical outcome. Overall, our findings delineate genomic changes that can be used in treatment management for patients with potentially malignant leukoplakia and OSCC patients with higher risk of lymphnode metastasis.

Publications

Journal

1. “Downregulation of Keratin 76 Expression during Oral Carcinogenesis of Human, Hamster and Mouse”, Srikant Ambatipudi*, Priyanka G. Bhosale*, Emma Heath, ManishkumarPandey, Gaurav Kumar,Shubhada Kane, AsawariPatil, Girish B. Maru, Rajiv S. Desai, Fiona M. Watt, Manoj B. Mahimkar,PLoS One, 2013; 8(7):e70688. (PMID:23936238)
   *Equal Contribution
2. “Low Prevalence of Transcriptionally Active HPV in Indian Head & Neck Squamous Cell Carcinoma and Leukoplakia”,Priyanka G. Bhosale, ManishkumarPandey, Rajiv S. Desai, AsawariPatil, Shubhada Kane, Kumar Prabhash, Manoj B. Mahimkar, Oral Surgery, Oral Medicine, Oral Pathology, Oral Radiology,2016; 122(5):609-618(PMID: 27765330)
3. “Chromosomal Aberrations and Gene Expression Changes Associated with the Progression of Leukoplakia to Advanced Gingivobuccal Cancer”, Priyanka G. Bhosale, SimonaCristea, SrikantAmbatipudi, Rajiv S. Desai, Rajiv Kumar, AsawariPatil, Shubhada Kane, Anita M. Borges, Alejandro A. Schäffer, NikoBeerenwinkel, Manoj B. Mahimkar, (Manuscript under review).
4. “Recurring Copy Number Gain at Chromosome 11q22 Plays an Important Role in Lymph Node Metastasis and Radioresistance in OSCC”. Priyanka G. Bhosale, SimonaCristea,ManishkumarPandey, Mickey Shah, AsawariPatil, Alejandro A. Schäffer, NikoBeerenwinkel, Manoj B. Mahimkar(Manuscript under preparation)

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205. Name : **Debika Banerjee**
Enrolment No. : MATH08201104003
Date of Award of degree : 22.03.17
Constituent Institute : Harish-Chandra Research Institute
Title : Some Results Related To Riesz Sum And K-Free Integers.

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206. Name : **Bibekananda Maji**
Enrolment No. : MATH08201104002
Date of Award of degree : 22.03.17
Constituent Institute : Harish-Chandra Research Institute
Title : A Study Of Some Lambert Series.

Publications

Journal

1. Length of an arithmetic progression represented by a binary quadratic form, Pallab Kanti Dey and R. Thangadurai, Amer. Math. Monthly, 2014, Vol. 121, no. 10, 932-936.
2. An analogue of Artin's primitive root conjecture, Pallab Kanti Dey and Balesh Kumar, Integers, 2016, Vol. 16, Paper No. A67.

3. Arithmetic progressions on $y^2 = x^3 + k$, Pallab Kanti Dey and Bibekananda Maji, J. Integer Sequence, 2016, Vol. 19, Article 16.7.4.
4. Diophantine equations concerning balancing and Lucas balancing numbers, Pallab Kanti Dey and S. S. Rout, Archiv der Mathematik, 2017, Vol. 108, no. 1, 29-43.
5. Elliptic curves with rank 0 over number fields, Pallab Kanti Dey, Funct. Approx. Comment. Math. 2017, DOI: 10.7169/facm/1585.

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207. Name : **Bhabyadarsan Sahoo**
Enrolment No. : PHYS01201204005
Date of Award of degree : 27.03.17
Constituent Institute : Bhabha Atomic Research Centre,
Title : High pressure investigations on carbides, oxides and nitrides.

Abstract

Discovery of various important pressure induced phase transitions and measurement of high pressure equation of state (EOS), shock Hugoniot, pressure dependent elastic constants and strength properties of materials have been proved very important in both applied and basis sciences. The present thesis attempts to understand various aspects of material behavior under high pressure – high temperature by resorting *ab-initio* static lattice and lattice dynamic calculations as a tool for investigations. In CdO, the comparison of enthalpies of NaCl type (B1) and CsCl type (B2) structures as a function of pressure suggests the B1to B2 transition at ~ 87GPa, in good agreement with experimental value of 90.6 GPa. Further, the analysis of elastic and the lattice dynamic instability of B1 and B2 structures and demonstrates that at ambient conditions, the B1 phase is stable elastically as well as lattice dynamically whereas the B2 structure is unstable both elastically as well as dynamically. Upon compression, the B2 structure emerges as elastically stable phase at ~ 38 GPa and lattice dynamically stable at ~ 55 GPa. The Hugoniot of CdO in B1 phase has been also determined. In carbides of transition metals ScC and YC, the theoretical calculation suggest the B1 phase of these materials will transform to primitive orthorhombic (Pmmn) structure instead of transforming to B2 phase that predicted by other studies. The transition pressure determined for this transition is ~ 80 GPa for ScC and ~30 GPa for YC. In TaC instead of Pmmn phase, the theoretical calculation predicts B2 structure at 472GPa. In UC, the theoretical calculation suggest at pressure of 20GPa, the B1 phase transforms to Pmmn phase but also identified the experimentally undetermined locations of U and C atoms in the high pressure phase. In ThC the comparison of enthalpies, derived for various phases using evolutionary structure search method in conjunction with first principles total energy calculations at several hydrostatic compressions, yielded a high pressure structural sequence of B1 → Pnma → Cmcm → B2 at hydrostatic pressures of ∼19 GPa, 36 GPa, and 200 GPa, respectively.. In CeN, the theoretical calculation predicts under high pressure predicts B1 → B10(P4/nmm) → B2 structural transitions at 53 and 200GPa instead of experimentally reported direct B1 to B2 transition at 65 GPa. To resolve this discrepancy the lattice dynamic calculations on these structures have produced that at ambient condition the B1 phase is dynamically stable, and B10 and B2 are unstable. At 60 GPa, however, the B1 phase becomes dynamically unstable and the B10 structure emerges as a dynamically stable phase whereas B2 still remains unstable.

Publications

Journal

1. “Prediction of new high pressure structural sequence in thorium carbide: A first principles study ” B. D. Sahoo, K. D. Joshi and Satish C. Gupta, **,** J. Appl. Phys.117, 185903 (2015).
2. “ Pressure effect on elastic, lattice dynamic and superconducting behavior of yttrium sulfide: A first principle study ” B.D. Sahoo, K.D. Joshi and Satish C. Gupta, J. Appl. Phys., 115, 123502-8 (2014).
3. “On equation of state , elastic, and lattice dynamic stability of bcc bismuth under high pressure :Ab-initio calculations” D. Mukherjee, B.D. Sahoo, K.D. Joshi and Satish C. Gupta, J. Appl. Phys., 115, 053702-7 (2014).
4. “ Structural, elastic and lattice dynamic stability of yttrium selenide (YSe) under pressure: A first principle study ” , B. D. Sahoo, K. D. Joshi and Satish C. Gupta, **,** J. Appl. Phys.116, 193504 (2014).
5. “Theoretical prediction of high pressure phase transition in ScC and YC: Ab initio calculations” B.D. Sahoo, K.D. Joshi and Satish C. Gupta, J. Appl. Phys 114, 053516 (2013).
6. “On Structural Stability of LaN Under High Pressure: ab-initio calculations” D. Mukherjee, B.D. Sahoo, K.D. Joshi and Satish C. Gupta, High Pres. Res., 33, 563 (2013).
7. “On the structural stability of CeN at high Pressure: Ab-initio calculations” B.D. Sahoo, K.D. Joshi and Satish C. Gupta, J. Appl. Phys., 113, 1935121-7 (2013).
8. “Ab-initio study on structural stability of uranium carbide” B.D. Sahoo, K.D. Joshi and Satish C. Gupta, J. Nucl. Mater, 437, 81 (2013).
9. “Ab-initio Calculations on structural, elastic and dynamic stability of CdO at high pressures” B.D. Sahoo, K.D. Joshi and Satish C. Gupta, J. Appl. Phys., 112, 0935231-6 (2012).
10. 10.“Thermo-physical properties of LiH at high pressures by ab initio calculations”, D. Mukherjee, B. D. Sahoo, K. D. Joshi, S. C. Gupta, and S. K. Sikka, J. Appl. Phys., 109, 103515 (2011).

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208. Name : **Subba Reddy Marri**
Enrolment No. : CHEM11201004008
Date of Award of degree : 29.03.17
Constituent Institute : National Institute of Science Education and Research,
Title : Investigation Of Open-Framework Metal Sulfates And Supercapacitors Based On Vanadium Chalcogenides-Rgo/Cnt Hybrids..

Publications

Journal

1. #Subba R. Marri, J. N. Behera, Synthesis, structure and photoluminescence properties ofamine-templated open-framework bismuth sulfates. *J. Solid state Chem*., 2014, *1*, 15-21.

2. #J. N. Behera, J. Bhattacharjee, S. Horike, Subba R. Marri, P. P. Dahiya, Synthesis and characterization of robust three-dimensional chiral metal sulfates. *RSC Adv.*, 2014, *4*, 50435-50442.
3. #S. Rath*, Subba R. Marri*, N. A. Lanzillo, S. Moshkalev, S. K. Nayak, J. N. Behera,Supercapacitors based on patronite–reduced graphene oxide hybrids: experimental and theoretical insights. *J. Mater. Chem*., 2015, *3*, 18874-18881. (*contributed equally)
4. S. Rath, Subba R. Marri, J. N. Behera, C. S. Rout, High-energy-density supercapacitorsbased on patronite/single-walled carbon nanotubes/reduced graphene oxide hybrids. *Eur. J. Inorg. Chem*., 2016, 259–265.
5. S. Bhowmick, S. Chakraborty, Subba R. Marri, J. N. Behera, N. Das, Pyrazine baseddonor tectons: synthesis, self-assembly and characterization. *RSC Adv*., 2016, *6*, 8992- 9001.

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209. Name : **Abhash Kumar Jha**
Enrolment No. : MATH11201104002
Date of Award of degree : 29.03.17
Constituent Institute : National Institute of Science Education and Research,
Title : Adjoint of Some Linear Maps Constructed Using Ranking-Cohen Brackets and Special Values of Certain Dirichlet Series.

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210. Name : **Lopamudra Das**
Enrolment No. : MATH11201104002
Date of Award of degree : 29.03.17
Constituent Institute : National Institute of Science Education and Research,
Title : Adjoint of Some Linear Maps Constructed Using Ranking-Cohen Brackets and Special Values of Certain Dirichlet Series.

Abstract

Understanding the role of Siah Proteins and its regulation during *Helicobacter pylori*-mediated gastric cancer is the primary objective of this thesis. Ubiquitin-mediated proteasomal degradation pathways control protein structure, function, assembly, localization as well as denaturation [1]. This pathway involves a series of enzymatic reactions catalyzed by a cascade of enzymes, *i.e*. E1 ubiquitin-activating enzymes, E2 ubiquitin-conjugating enzymes and E3 ubiquitin-ligase enzyme that causes transfer of E2-linked ubiquitin to a Lys residue of a targeted protein. The tagged proteins get degraded either by the 26S proteasome or by the lysosome [2]. The importance of E3 ligase lies in that it confers specificity to ubiquitination by identifying the target proteins and thus acts as a mediator for transfer of ubiquitin from an E2 ubiquitin-conjugating enzyme to the target protein [1]. The really interesting new gene (RING) family of E3 ubiquitin ligases play crucial role in regulating cancer progression and metastasis for adenocarcinoma [3]and have drawn attention as potential drug targets [4]. The evolutionarily conserved seven in absentia homolog (Siah) proteins belong to the RING family of E3 ubiquitin ligases. So far three *siah*genes have been identified in human *i.e*. *siah-1*, *siah-2* and *siah-3* [5, 6]. There are no reports on the role of Siah3 in cancer progression whereas the other two Siah proteins were shown to interact with and regulate the stability of multiple factors involved in oncogenesis including prolyl hydroxylases, β-catenin, NUMB, tumour necrosis factor receptor 2–associated factor and Sprouty[7-11]. Induced expression of Siah proteins in various cancers supports their tumour-

promoting role [12-16]. Moreover, elevated level of Siah2 expression in breast, prostate and liver cancer cells has been linked with malignancy and cancer invasiveness [12, 13]. But limited number of studies are available that explored role of Siah proteins in gastric cancer progression. Gastric cancer is the most common malignant cancer and is a leading cause of cancer-related mortality. Due to its complex initiation and progression mechanism it is generally diagnosed at later stages when the cancer has already started metastasizing [17, 18]. Infection with *H. pylori* is the prime factor responsible for gastric cancer. *H. pylori* colonizes nearly half of the world population and has been recognized as a type I carcinogen for gastric cancer [19]. Therefore, understanding the role of Siah proteins in the complex process of gastric cancer progression and metastasis is imperative in the *H. pylori*-infected gastric epithelium. It is interesting to identify transcription factors regulating expression of Siah proteins as there are very few reports. So far, Siah1 has been mainly reported as a tumour-suppressor but Siah2 has been portrayed as a tumour-promoting agent. This discrepancy in function suggests that a Siah1 and Siah2 might have different set of downstream target proteins modulating various signalling network [20]. Hence, identifying the regulation of Siah protein expression and in-depth understanding of their functions during gastric cancer progression are important.This thesis work focuses to understand the role of Siah proteins and their regulation during *H. pylori*-mediated gastric cancer progression. This thesis has been structured into five chapters and contents of each chapter have been discussed briefly as follows.

Publications

Journal

1. Regulation of Noxa-mediated apoptosis in *Helicobacter pylori*–infected gastric epithelial cells. SuvasmitaRath, Lopamudra Das, ShrikantBabanraoKokate, B M Pratheek, SubhasisChattopadhyay, ChandanGoswami, RanajoyChattopadhyay, Sheila Eileen Crowe, Asima Bhattacharyya. *FASEB J. 2015 Mar; 29(3): 796-8*
2. Cobalt chloride-mediated protein kinase Cα (PKCα) phosphorylation induces hypoxia-inducible factor 1α (HIF1α) in the nucleus of gastric cancer cell. SuvasmitaRath, AdityaAnand, NilabhGhosh, Lopamudra Das, ShrikantBabanraoKokate, Pragyesh Dixit, SwetapadmaMajhi, Niranjan Rout, Shivaram Prasad Singh, Asima Bhattacharyya. *BiochemBiophys Res Commun.* 2016 Feb 26; 471(1): 205-12
3. *ETS2 and Twist1 promote invasiveness of *Helicobacter pylori*-infected gastric cancer cells by inducing Siah2. Lopamudra Das, ShrikantBabanraoKokate, SuvasmitaRath, Niranjan Rout, Shivaram Prasad Singh, Sheila Eileen Crowe, Asish K Mukhopadhyay, Asima Bhattacharyya. *Biochem. J.* (2016) 473, 1629–1640
4. Inhibition of Histone/Lysine Acetyltransferase Activity by CTK7A Selectively Kills Hypoxic Gastric Cancer Cells. SuvasmitaRath, Lopamudra Das, ShrikantBabanraoKokate,NilabhGhosh, Pragyesh Dixit,Niranjan Rout, Shivaram P Singh, SubhasisChattopadhyay, Hassan Ashktorab, Duane T Smoot, Mahadeva M Swamy, Tapas K Kundu, Sheila E Crowe, Asima Bhattacharyya. *Int J Biochem Cell Biol.* 2017 Jan;82:28-40

211. Name : **Trisha Nath**
Enrolment No. : PHYS10201104002
Date of Award of degree : 29.03.17
Constituent Institute : Institute of Mathematical Sciences,
Title : Phase behaviour and ordering in hard core lattice gas models.

Abstract

Systems of particles that interact only through excluded volume interactions are minimal models to study entropy-driven phase transitions. In this thesis we study in detail two hard core lattice gas models on the square lattice, (1) The k-NN model which is the discrete version of the hard disc system in two dimensions and (2) hard rectangles and squares.In the k-NN model the first k nearest neighboring lattice points of a particle are excluded from being occupied by another particle. In the 4-NN model, using Monte Carlo simulations we find the existence of two continuous transitions with increasing density -- the first from disordered to sublattice-ordered phase and the second from sublattice-ordered to columnar-ordered phase. We further analytically rationalize the existence of multiple transitions by high-activity series expansion. Extending the argument, we conjecture that if the model satisfies (i) the high density phase is columnar and (ii) sliding instability is present in only a fraction of the sublattices, then the system will show multiple transitions. We verify the same in k-NN models with k=6, 7, 8, 9, 10, 11 using Monte Carlo simulations. The conjecture reduces to determining, for a given k greater than 5, whether the high density phase has columnar order at close packing. Finding out close packing structure for k-NN with k up to 820302, we show that there are only eighteen values of k, all less than k = 4134, that show columnar order, while the others show solid-like sublattice order.We further analytically study the columnar phase in classical 2x2 hard-square lattice gas and mxd hard rectangles on square lattice. By deriving the exact expression for the first d + 2 terms in the free energy expansion, we obtain lower bounds for the critical density and activity for nematic-columnar transition. To obtain a better estimate of the critical parameters of the transition, we estimate the interfacial tension between two phases with different columnar order in a system of 2xd hard rectangles. Setting the interfacial tension to zero, we obtain a condition for the limit of stability of the columnar ordered phase. For all values of d, the critical parameters obtained are in good agreement with numerical data.

Publications

Journal

1. The high density phase of the k-NN hard core lattice gas model Trisha Nath and R. Rajesh *J. Stat. Mech., 2016,* 7, 073203.
2. Stability of columnar order in assemblies of hard rectangles or squares Trisha Nath, Deepak Dhar and R. Rajesh *Europhys. Lett., 2016,* 114, 10003
3. High-activity expansion for the columnar phase of the hard rectangle gasTrisha Nath, Joyjit Kundu and R. Rajesh *J. Stat. Phys., 2015,* 160, 1173
4. Multiple phase transitions in extended hard-core lattice gas models in two dimensions Trisha Nath and R. Rajesh *Phys. Rev. E, 2014,* 90, 012120

212. Name : **Upayan baul**
Enrolment No. : PHYS10201104006
Date of Award of degree : 29.03.17
Constituent Institute : Institute of Mathematical Sciences,
Title : Influence of the presence of solutes on the structural and dynamical properties of lipid membranes and water.

Abstract

In this thesis, titled *Influence of the presence of solutes on the structural and dynamical properties of lipid membranes and water*, we report classical all-atom molecular dynamics (MD) simulation studies of two biological solvents, namely- phospholipid bilayers and water, and their interactions with flexible, amphiphilic, polycationic antimicrobial polymers and dissolved salts (ions) respectively.

For methacrylate polymers characterized by backbone amphiphilicity, we study the interactions of polymer aggregates with multiple model lipid membranes which include models for both mammalian and microbial membranes. We conclusively show that the polymers impact the structural properties of the microbial membrane models, with minimal effect on a mammalian one. For a model of *E. Coli* membrane, we suggest a mode of antimicrobial activity through polymer induced demixing of lipid species, and associated phase boundary defects. We also report that the flexible methacrylate polymers with no built-in facial amphiphilicity are capable of acquiring facial amphiphilicity in their membrane partitioned phase. For side-chain amphiphilic polymers, in collaboration with experiments, we show that the hydrogen bonding ability of polymers can impact their antimicrobial activity.Our studies reveal the effect of both monovalent and divalent cations on the long-range dipolar orientational correlations in liquid water. Based on the observations, the ambiguous classification of ions as structure makers and breakers is challenged. The importance of the results is discussed in the context of hydrophobic aggregation. Finally, using a new selection criteria for water molecules, we show that strongly solvated ions such as Mg^{2+} can induce reorientational slowing of water molecules beyond the first ion solvation shells. The slow water molecules are further shown to be de-localized. The results explain the contrasting observations from a class of experiments (FS-IR) and prior numerical simulations.

Publications

Journal

1. Interaction of multiple biomimetic antimicrobial polymers with model bacterial membranesUpayan Baul, Kenichi Kuroda and Satyavani Vemparala *J. Chem. Phys., 2014,* 141, 084902
2. Ion hydration and associated defects in hydrogen bond network of water: Observation of reorientationally slow water molecules beyond first hydration shell I aqueous solutions of MgCl$_2$Upayan Baul and Satyavani Vemparala*Phys. Rev. E, 2015,*91, 0121
3. Effect of simple solutes on the long range dipolar correlations in liquid water Upayan Baul, J. Maruthi Pradeep Kanth, Ramesh Anishetty and Satyavani Vemparala *J. Chem. Phys., 2016,* 144, 104502
4. Isosteric substitution in cationic-amphiphilic polymers reveals an important role for hydrogen bonding in bacterial membrane interactions Divakara S. S. M. Uppu, Mohini M. Konai, Upayan Baul, Priyank Singh, Tjalling K. Siersma, Sandip Samaddar, Satyavani Vemparala, Leendert W. Hamoen, Chandrabhas Narayana and Jayanta Haldar *Chem. Sci., 2016,*7, 4613

213. Name : **Soumyadeep Bhattacharya**
Enrolment No. : PHYS10201004008
Date of Award of degree : 29.03.17
Constituent Institute : Institute of Mathematical Sciences,
Title : Role of Topological Defects in Breaking and Enhancing Discrete Symmetries.

Abstract

Phase transitions accompanied by spontaneous breaking of continuous symmetries have been studied extensively in condensed matter and high energy physics. In this thesis we investigate the spontaneous breaking of discrete symmetries, specifically in spin models with three-fold, four-fold and higher discrete symmetries. We show that an interplay between the topological defects - domainwalls and vortices - in these models drives the discrete symmetry to be completely broken, partially broken and even enhanced to a continuous U(1) symmetry. We show that in two dimensions, percolation of domain walls drives a transition from a symmetry broken ordered phase to a symmetry enhanced quasi long range ordered phase which, in turn, undergoes a transition to the symmetry restored disordered phase when vortices proliferate. We highlight a flaw in the standard method for calculating winding numbers and propose a new method which correctly identifies vortices. We show that suppression of vortices in models with even number of states leads to an intermediate partially ordered phase and that additional suppression of domain walls, separating opposite spin states, is required to manifest the symmetry enhanced phase. We show that spin models with three or higher number of states exhibit a partial symmetry broken phase instead of symmetry enhanced phase in three dimensions as individual types of domain walls are able to percolate on their own. We also obtain a variety of phases by suppressing defects belonging to subgroups of the model's symmetry. Upon enhancing the formation of vortices instead of suppressing them, we obtain a vortex-antivortex lattice phase in two dimensions and a vortex condensate phase in three dimensions.

Publications

Journal

1. “Quasi-Long-Range Order and Vortex Lattice in the Three-State Potts Model” Soumyadeep Bhattacharya and Purusattam Ray*Physical Review Letters,* 2016, 116, 097206.

Conference Proceedings

a. “Emergence of U(1) symmetry in Z(q) clock model”Soumyadeep Bhattacharya and Purusattam Ray*AIP Conference Proceedings*, 2012, 1447, 91

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214. Name : **Gaurav Rattan**
Enrolment No. : MATH10201005005
Date of Award of degree : 29.03.17
Constituent Institute : Institute of Mathematical Sciences,
Title : Some Geometrical and Vertex-Partitioning Techniques for Graph Isomorphism.

Abstract

The Graph Isomorphism Problem consists of the following natural question: given two graphs, are they isomorphic? In other words, does there exist an adjacency-preserving bijection between the vertex sets of the two graphs? A multitude of theoretical ideas and techniques have found application to the Graph

Isomorphism Problem. In this thesis, we explore some non-group-theoretic approaches to Graph Isomorphism. Given two sets A and B of n points in a k-dimensional Euclidean space, does there exist a distance-preserving bijection between them? Formally called Geometric Graph Isomorphism, this problem is a geometric analogue of Graph Isomorphism. In our study, we consider point-sets with rational entries. Using techniques from geometry and lattices, we obtain a ~O(2O(k2)) time FPT algorithm for this problem (the ~O notation hides factors which are polynomial in input size). Here, the dimension k of the underlying space is the parameter of interest. We then consider the problem of computing canonical forms for geometric point-sets in Qk. We obtain a ~O(kO(k)) time procedure for geometric graph can- onization. The canonization procedure immediately implies a faster ~O(kO(k)) running time FPT algorithm for GEOM-GI. We also briefly consider the isomorphism problem for other lp metrics (the case p = 2 is Euclidean). The one-dimensional version of the Weisfeiler-Leman algorithm is commonly known as Color-Refinement, or naive vertex-classification. Color-Refinement is a classical procedure used to distinguish non-isomorphic graphs. This motivates the following natural question: what is the exact scope of applicability of color-refinement? We call a graph G amenable if color-refinement successfully distinguishes G from any other non-isomorphic graph H. We obtain a polynomial time algorithm for testing whether a given graph is amenable. In fact, we show that this problem is complete for the complexity class P, under logspace reductions. Continuing this theme, we examine the power and limitations of convex optimization techniques for GI. In this context, there exists a very natural class of graphs called compact graphs. The isomorphism problem for compact graphs can be efficiently solved using linear programming methods. Can we give a characterization for the class of compact graphs? In our work, we show that the class of compact graphs contains the class of amenable graphs. Exploring this connection further, we study a strict hierarchy of graph classes based on structural, group-theoretic and algorithmic properties of graphs with respect to isomorphism testing.

Publications

Journal

1. V. Arvind, G. Rattan. The parameterized complexity of Geometric GraphIsomorphism. Algorithmica, 75:2, 258{276, 2016.
2. V. Arvind, J. K obler, G. Rattan, O. Verbitsky. Graph Isomorphism, Color Refinement, and Compactness. Computational Complexity. 1{59, 2016.

List of Publications in Conferences

1. V. Arvind, G. Rattan. The parameterized complexity of Geometric Graph Isomorphism. In Proceedings of 9th International Symposium on Parame- terized and Exact Computation, (IPEC 2014), pp. 51{62, 2014.
2. V. Arvind, J. K obler, G. Rattan, O. Verbitsky. On the power of color refinement. In Proceedings of the 20th International Symposium on Funda-mentals of Computation Theory (FCT), pp. 339{350, 2015.
3. V. Arvind, J. K obler, G. Rattan, O. Verbitsky. On Tinhofer's linear programming approach to isomorphism testing. In Proceedings of the 40th International Symposium on Mathematical Foundations of Computer Sci- ence (MFCS), pp. 26{37, 2015.

215. Name : **Amit Kumar**
Enrolment No. : PHYS02201004019
Date of Award of degree : 29.03.17
Constituent Institute : Indira Gandhi Centre for Atomic Research,,
Title : Sodium Metal Aerosol Characterization In Cover Gas Region.

Abstract

In a SFR, the sodium metal aerosol characteristics present in the cover gas region is important to understand the heat and mass transfer to the roof top and side wall, visibility of cover gas region, design of purification system efficiency, aerosol deposition to roof top and its penetration, convection velocity in cover gas region and fission product scavenging by these aerosols. Development of theoretical models and their verification on specific experimental results remain necessary to determine/estimate sodium aerosol mass concentration and sodium aerosol size distribution and their effect on thermal radiation in sodium aerosol filled areas. The sodium metal aerosol characteristics in cover gas region is determined for sodium pool temperature ranges from $250^{o}C$ - $550^{o}C$ taking into account of spatial variation within the cover gas space. Besides, the effects of geometric dimension of the cover gas region and gamma radiation on sodium metal aerosol characteristics are studied. A theoretical model is developed to predict sodium metal aerosol characteristics in cover gas region and validated with experimental results. The study consists of (i) development of characterization technique for sodium metal aerosols in cover gas region without exposing the aerosol to atmosphere and its validation, (ii) Measurement of temperature profile in the cover gas region, (iii) Development of empirical relation for estimation of bulk cover gas temperature, (iv) sampling and characterisation of sodium metal aerosols at three different height of the cover gas region and in different geometry and (v) development of theoretical model. The results showed that the sodium metal aerosol size (MMD) and mass concentration is rages from 1.5 µm to 16 µm and 0.026 g/m^3 to 35.55 g/m^3 i.e. increases with increase of sodium pool temperature for a given geometry. The MMD of sodium metal aerosol size is larger and mass concentration is more near the sodium pool compared to that of the middle level of cover gas region and near the roof for a given geometry. The MMD of sodium metal aerosol increases and mass concentration of sodium aerosol decreases with the increase of aspect ratio (L/D L – height and D – diameter) of cover gas region. The experiments are conducted by exposing the region with gamma radiation field and it is found that, the MMD of sodium metal aerosol is found to be higher and mass concentration is found to be less in the presence of gamma field when compared to that of without gamma field condition.The study is found to be useful for prediction of sodium metal aerosol characteristics in cover gas region for aspect ratio $0.55 \leq L/D \leq 4.52$ and for the sodium pool temperature $250^{o}C \leq T_p \leq 550\ ^{o}C$. The model is also used to predict the sodium aerosol concentration in the space between Main vessel and Safety vessel of PFBR in the event of leakage of sodium from the main vessel in order to evaluate the performance of sodium aerosol detector which is going to be installed in PFBR. In continuation of this work it is proposed to conduct experiment in FBTR for characterising of sodium metal aerosol in cover gas region.

Publications

Journal

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2. "Development and validation of methodology for characterization of sodium aerosols in cover gas region", Amit Kumar, Subramanian V., Baskaran R., Krishnakumar S., Chandramouli S. and Venkatraman B., Aerosol and Air Quality Research, 2014, Vol. 14, 1534-1541.

3. “Characterization of Sodium Aerosol in Cover Gas Region of SILVERINA Loop”, Amit Kumar, Subramanian V., Krishnakumar S., Baskaran R., Chandramouli S. and Venkatraman B., Aerosol and Air Quality Research, 2015, Vol.15, 1813-1822.
4. “Size Evolution of sodium combustion aerosol with various RH%”, Amit Kumar, Subramanian V., Baskaran R., and Venkatraman B., Aerosol and Air Quality Research, 2015, Vol.15, 2270-2276.
5. “Studies on Geometrical effect on sodium aerosol characteristics in cover gas region”, Amit Kumar, Subramanian V., Baskaran R., Krishnakumar S., Chandramouli S. and Venkatraman B., Aerosol and Air Quality Research, 2016, Vol.16, 1832-1840.

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216. Name : **Chanchal Ghosh**
Enrolment No. : PHYS02201004021
Date of Award of degree : 29.03.17
Constituent Institute : Indira Gandhi Centre for Atomic Research,,
Title : Phase Stability And Microstructural Evolution In V-Ti-Cr System Using Phase Contrast, Haadf Imaging And Electron Spectroscopy.

Abstract

V-Ti-Cr alloys are potential candidate materials for advanced engineering applications such as first-wall blanket material in fusion based reactors as well as for hydrogen storage application. However the phase transformation behaviour of the constituent binaries and the ternary V-Ti-Cr system are not well understood in literature. Based on Miedema model several compositions of V-Ti-Cr alloys have been identified and prepared by vacuum arc melting – V-4Ti-4Cr from the V rich corner of the ternary system to study stability of the solid solution phase, V-39Ti-54Cr from the Ti-Cr rich side of the diagram to study stability of amorphous / intermetallic phases, V-50Ti and V-40Ti-20Cr from the V-Ti rich side of the alloy system to study presence of a miscibility gap. These calculations have further been supported by ThermoCalc model and Pettifor structure map approach. Microstructural and microchemical evolution in this set of alloys has been studied using advanced transmission electron microscopy (TEM) techniques of phase contrast (with multislice simulation), STEM-HAADF, XEDS, EFTEM and EELS. Detailed TEM studies confirm the stability of a *bcc* solid solution phase at the V-rich corner of the V-Ti-Cr ternary system. For a ternary extension of the binary $TiCr_2$ Laves phase, formed by addition of V to the extent of 7 atom%, zero loss phase contrast microscopy has been carried out to distinguish the atomic columns unambiguously. Results indicate that Ti and Cr atoms are not imaged simultaneously at all thickness – defocus combinations; this is further confirmed by phase contrast image simulations. The difference in the channelling behaviour of Ti and Cr atomic columns convoluted with the instrument CTF results in the disappearance of bright contrast for specific atom sites in the unit cell. Comparisons of the experimental and simulated electron intensity profiles supported by first principles calculations confirm that V preferentially substitutes Ti rather than Cr from the regular lattice sites. This further confirms, V-doped $TiCr_2$ exists as a pseudo-binary Laves phase with a modified stoichiometry of $(Ti,V)Cr_2$. For binary V-Ti alloys, the prediction of a phase separation tendency that reduces with addition of Cr by thermodynamic calculations is confirmed. . Lamellar nanostructured domains with coherent interfaces seen in the phase contrast imaging of V-50Ti and V-40Ti-20Cr alloys, indicative of a phase separation event. STEM-HAADF studies indicate the compositional modulation normal to the lamellar domains and further examined through STEM-XEDS and STEM-EELS techniques. It is apparent from the results that the phase separation is essentially a binary event involving only Ti and V - Cr is homogeneously distributed. The initial composition fluctuation wave in binary V-50Ti alloy is of wavelength ~ 4-5 nm. Gradually another wave with wavelength ~ 18-20 nm initiates and finally this alone persists. Subsequent TEM studies suggest that the composition modulation is governed by a spinodal decomposition mechanism and not by diffusion and growth kinetics. As a result of the phase separation, a Ti rich domain evolves in the matrix, which becomes thermodynamically viable for the nucleation of ω phase. HRTEM images as recorded

along <1 1 0> and <-1 1 3> zone axis of the *bcc* phase confirms that in most of the cases the collapse is partial, yielding the trigonal ω phase. HRTEM analysis along with image simulation further shows the systematic absence of the bright atom contrast for the corner atoms of the ω phase. A combination of phase contrast and Z contrast microscopy coupled with electron spectroscopy imaging, phase contrast image simulation and atomic structure modelling have been successfully analyse the materials related issues of V-Ti-Cr alloys which is otherwise not possible through any of the conventional techniques.

Publications

Journal

1. "Synthesis and structural characterization of V-4Ti-4Cr alloy", C Ghosh, J. Basu, S. Khan, R. Divakar, E. Mohandas, M. Vijayalakshmi, *Trans. Ind. Inst. Met.,* 2013, 66(4), 381-385.
2. "Structure imaging and Vanadium substitution in cubic TiCr2 Laves phase"C. Ghosh, V. Sharma, J. Basu, R. Divakar, E. Mohandas, , *Philos. Mag.,* 2015 95:22, 2403-2426.
3. "Alloy design and microstructural evolution in V-Ti-Cr alloys", C. Ghosh, J. Basu, R. Divakar, E. Mohandas, *Mater. Characterization,* 2015, 106, 292- 301.
4. "Phase and microstructure evolution in V-Ti-(Cr/W) alloys", C. Ghosh, J. Basu, R. Divakar, E. Mohandas, *Mater. Today: Proc.* 2016, 3(9), 2920-2925.
5. "Phase separation and ω transformation in binary V-Ti and ternary V-Ti-Cr alloys", C. Ghosh, J. Basu, R. Divakar, E. Mohandas, *Acta Mater.*, 2016, 121, 310-324.
6. "Microstructural and microchemical studies of phase stability in V-O solid solution", C. Ghosh, A. Singh, J. Basu, R. Divakar, E. Mohandas, *Mater. Characterization,* 2017, 124, 129-135.

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217. Name : **Ekjot Kaur**
Enrolment No. : LIFE09201104002
Date of Award of degree : 29.03.17
Constituent Institute : Tata Memorial Centre
Title : Role of chromatin and DNA Damage repair pathway in Glioblastoma Multiforme.

Abstract

In this study, we address the fundamental issue of radiation resistance in Glioblastoma Multiforme (GBM) a highly malignant form of brain tumor. However, because of the inaccessibility to the inherently resistant cells that are responsible for recurrence in GBM, our understand ding of thesurvival strategies adopted by the tumor cells has been limited. To circumvent this problem, we recapitulated clinical scenario of GBM resistance in a cellular model developed from fresh naïve primary GBM patient samples and cell lines. Using our model, we show that upon lethal dose of radiation, small percentage of GBM cells survive, are non-apoptotic and transiently become non- proliferative. They are arrested in G2/M phase of cell cycle mediated by inhibitory phosphorylation of Cdk1(Y15) and p21. Surprisingly, we find although non -proliferative, these radiation resistant cells (RR) are highly motile and undergo homotypic cell-cell fusions at high frequency to form multinucleated and giant cells (MNGCs). Cell fusion leads to the induction of senescence as seen by β-galactosidase staining and high expression of SASPs (senescence associated secretory proteins) is also observed. SASPs provide survival and proliferation signals to the cells in an autocrine manner and thus allow RR cells to regrow and give rise to recurrent cells. We also find enhanced expression of anti-apoptotic genes BIRC3 and Bcl-xL mRNA as well as activeAKT in RR cells which synergistically regulate the apoptosis.

Importantly, we show that the duration of the resistant cell formation is associated with poor prognosis in GBM. Since DNA damage repair (DDR) pathway plays a significant role in maintaining genomic stability, we wanted to understand how MNGCs modulate their DDR pathway. We show that MNGCs activate ATM-Chk2 or ATR-Chk1-RPA2 axis, repairing their DNA by Non homologous End Joining (NHEJ) pathway and not by Homologous Recombination. Given the association of DDR and histone methylations, we found up-regulation of H3K36me2 and SETMAR methyltransferase predominantly in the RR cells displaying a euchromatin architecture.H3K36me2 is known to enhance recruitment of NHEJ repair components including Ku80. Accordingly, we demonstrate that mutating H3.3 at lysine 36 or knockdown of SETMAR in RR cells decreased the NHEJ repair response at the DSB site and alleviated survival of resistant cells. Additionally, inhibition of NHEJ pathway using DNA-Pk inhibitor NU7026 decreased the survival capacity of radiation resistant cells. In summary, our data provide a mechanistic explanation and novel insights into an unexplored multi-step process of radiation survival and recurrence in Glioblastoma. We identified novel homotypic cell fusions of resistant Glioma cells which modulate histone methylation, promoting NHEJ-driven repair of DSBs. These are novel mechanisms that facilitate survival and recurrence, thereby generating a rationale for developing combinatorial therapies.

Publications

Journal

1. “Radiation-induced homotypic cell fusions of innately resistant glioblastoma cells mediate their sustained survival and recurrence”. Kaur E, Rajendra J, Jadhav S, Sridhar E, Goda JS, Moiyadi A and Dutt S. *Carcinogenesis*,2015Jun; 36(6):685-95. doi: 10.1093/carcin/bgv050.
2. “Unique spectral markers discern recurrent Glioblastoma cells from heterogeneous parent population”. Kaur E,Sahu A, Hole A, Rajendra J, Chaubal R, Gardi N, Dutt A, Moiyadi A, Krishna CM and Dutt S. *Sci Rep.*, 2016 May; 6, 26538. doi: 10.1038/srep26538 (2016).

Conferences:

1. Ekjot Kaur, Gauri Patade, Sneha Berry and Shilpee Dutt. “Surviving Genotoxic Stress” poster presentation at “at XXXVI All India Cell Biology Conference -2012 and International Symposium on SARGI: 17-19th November, 2012,Mumbai, India.
2. Ekjot Kaur, Shailesh Jadhav, Sneha Berry, Gauri Patade and Shilpee Dutt “Polyploidy: a survival mechanism against ionizing radiation in Glioblastoma”. Poster presentation at “32nd Convention of Indian Association for Cancer Research Emerging Trends in Cancer research: Road to prevention & cure & International Symposium on: Infection and Cancer” (IACR-2013-February 13 -16 2013) under Shri Rambhau Kulkarni and Shri Rajnikant Baxi award category, New Delhi, India.
3. Ekjot Kaur, Jacinth Rajendra, Shailesh Jadhav, Gauri Patade and Shilpee Dutt “Multinucleated giant cells formed by cell - cell fusion post radiation are cause of resistance and relapse in Glioblastoma”. Oral presentation award under Shri Sitaram Joglekar category at “33rd Annual Convention of Indian Association for Cancer Research (IACR)” 13-15,2014 February, 2014, Kerala, India.
4. Ekjot Kaur, Shailesh Jadhav, Aliasgar Moiyadi, Jayant S Goda and Shilpee Dutt “Radiation induced homotypic cell fusions of resistant cells form multinucleated giant cells: cause of sustained survival and recurrence in glioblastoma” platform presentation at “ISNOCON2015, Kochi” 26th-28th March 2015,Kochi, India.

5. Ekjot Kaur Jacinth Rajendra, Sanket Shah, Jyothi Nair, Ankit Khushwaha, Aliasgar Moiyadi, Shilpee Dutt, “Radiation induced Multinucleated Giant Cells: a novel therapeutic target to prevent survival and relapse of Glioblastoma” poster presentation during 106th Annual Meeting of American Association for Cancer Research (AACR-2015,April 18-22) in Philadelphia, PA, USA.
6. Ekjot Kaur, Jyothi Nair,Ankit Kushwaha, Akshat Shetty, Anurag Srivastava, Aliasgar Moiyadi , Shilpee Dutt“A novel mechanism of homotypic cell fusion promote formation of Glioma resistance cells facilitated by NHEJ driven repair”Selected amongst top 12 abstracts for oral presentaionat 75th Tata Memorial Centre Platinum Jubilee Conference, 26-28th Feb 2016, Mumbai, India.

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218. Name : **Pratik Chandrani**
Enrolment No. : LIFE09201104003
Date of Award of degree : 29.03.17
Constituent Institute : Tata Memorial Centre
Title : Discovery of Potential Therapeutic Targets in Human Cancer: A Functional Genomics Approach.

Abstract

Several human diseases, most notably cancer research has seen unprecedented progress in past decade due to identification of various molecular alterations driving tumor growth and development of highly specific therapeutic solutions targeting these molecular alterations. Several global consortia based projects have been initiated to profile large number of tumor genomes to identify therapeutically exploitable genomic alterations. These findings have revealed promising preliminary results in clinical practice such as Herceptin for breast cancer, Imatinib for leukemia, Erlotinib for lung cancer etc. that are unfortunately primarily restricted to developed nations. On the other hand, to generate and utilize these resources has been deterrent for the developing world due to the lack of appropriate infrastructure, resources and technical expertise requirement. As an attempt to circumvent the problem and help the wider community to tap the knowledge present in vast genomic data, my thesis focuses on following three functional aspects of the cancer genome as detailed below: 1) Generate a landscape of therapeutically relevant alterations using high throughput sequencing platform in human lung adenocarcinoma samples of Indian origin. In brief, I split my study design to sequence a smaller set of 45 samples by nextgenerationsequencing as the discovery set. Next, the mutations found werespecifically genotyped in a larger validation set of 363 samples using massspectrometrybased genotyping. This study led to establishment of the firsttherapeutically relevant landscape of alterations in lung adenocarcinoma of Indianorigin. This study also led to the identification of novel recurrent mutations infibroblast growth factor receptor 3 (*FGFR3*) which were validated to be oncogenicand sensitive to pharmacological inhibition using *in-vitro* and *in-vivo* approaches.

Publications

Journal

1. Chandrani P*, Prabhash K.*, Choughule A, Prasad R, Sethunath V, Ranjan M,Aich J, Dhamne H, Iyer D, Upadhyay P, Sundaram P, Mohanty B, Chandna P,Kumar R, Joshi A, Noronha V, Patil V, Ramaswamy A, Karpe A, Thorat R,

   Chaudhary P, Ingle A, Dutt A. Drug-sensitive FGFR3 mutations in lung adenocarcinoma. *Annals of Oncology*. 2016 Dec 19. pii: mdw636. doi: 10.1093/annonc/mdw636. PubMed PMID: 27998968 [Epub ahead of print].

2. Chandrani P*, Upadhyay P*, Iyer P, Tanna M, Shetty M, Raghuram GV, Oak N, Singh A, Chaubal R, Ramteke M, Gupta S, Dutt A. Integrated genomics approach to identify biologically relevant alterations in fewer samples. *BMC Genomics*. 2015 Nov 14;16(1):936. doi: 10.1186/s12864-015-2138-4. PubMed PMID: 26572163; PubMed Central PMCID: PMC4647579.
3. Chandrani P*, Kulkarni V*, Iyer P, Upadhyay P, Chaubal R, Das P, Mulherkar R, Singh R, Dutt A. NGS-based approach to determine the presence of HPV and their sites of integration in human cancer genome. *Br J Cancer*. 2015 Jun 9;112(12):1958-65. doi: 10.1038/bjc.2015.121. Epub 2015 May 14. PubMed PMID: 25973533; PubMed Central PMCID: PMC4580395.

Section –IV

Titles of completed M.Tech and M.Sc.(Engg.) dissertations during 2016-17

S. No.	Name	Degree	DOAPD	Thesis Title
1	Rahul Tripathi	M.Tech	07.06.16	Effect of Overload and Under Load on the Fatigue Crack Growth Behaviour of Carbon Steel Piping Material
2	Ankur Chowdhury	M.Tech	07.06.16	Design of IGBT Based Trigger Circuit for Simultaneous Triggering of Multiple Parallely Placed Ignitrons for Pulsed Power Applications
3	Rakesh Chouhan	M.Tech	07.06.16	Natural Circulation Studies in Molten Fluoride Salt Loop
4	Krishna Pal Namdeo	M.Tech	07.06.16	Modeling of Coupled heat and mass Transfer in Multi-Phase Desublimer for Different Designs
5	Chandrajeet Singh Chauhan	M.Tech	28.06.16	Sensitivity Analysis and Optimization of Swirl Injector System
6	Akhila V.R (AMD, Hyd.)	M.Tech	19.07.16	Lithological Structural and Geochemical Studies in and Around Garadih-Hitku-Patharchaki Area,. Central singhbhum Shear Zone to Understand the Role of soda Metasomatism in Uranium Mineralisation
7	Aneesh V.J(AMD, Hyd.)	M.Tech	19.07.16	Characterization of Unconformity and the Control f Uranium Mineralization in Karichhapar Area, Raigarh District, Chattisgarh
8	Debasish Roy (AMD, Hyd.)	M.Tech	19.07.16	Study of deformation , kinematics and Aspect of Metallogenesis along Gogi-Kurlagere Fault, Yadgir District, Karnataka, India
9	Junaid Ahmad (AMD, Hyd.)	M.Tech	19.07.16	Characterization of Sediments of Bortalao Formation from Dhara Area, Rainandgaon District, Chhatisgarh with Special Reference to its Uranium Potential
10	Marati Ruthvik (AMD, Hyd.)	M.Tech	19.07.16	Geological Mapping, Radiometric Survey and Sampling to Evaluate the Nature and Control of Uranium Mineralization in Bhojgarh-Gurha-Kakrana Areas, Jhunjhunu Dist., Rajasthan
11	Bolloju Priyatham Kumar (AMD, Hyd.)	M.Tech	19.07.16	Rare Metal and Rare Earth Bearing Granite Pegmatites with Special Emphasis on Petro-Mineralogical Studies Along Kolabira-Dhubenbudrenglol-Laida-Dhengorjor-Kira-Tract, Jharsuguda & Sambalpur Districts, Odisha
12	V.D.Rajesh Nagala (AMD, Hyd.)	M.Tech	19.07.16	Geogical Structural and Petromineralogical Controls of Uranium Mineralization in Albitised rocks of NDFB in Part of Haryana
13	Shivam Shrivastava (AMD, Hyd.)	M.Tech	19.07.16	Geological Mapping and Petrological Study of Granites South of Achola Fault Zone to Understand the Nature and Control of Uranium Mineraization, Yadgir District, Karnataka
14	Santu Patra (AMD, Hyd.)	M.Tech	19.07.16	Petromineralogical and Geochemical Study to Characterize Uranium Mineralization in Dupu and Surrounding Areas, West Siang District, Arunachal Pradesh

15	Hiranmoy Mondal (AMD, Hyd.)	M.Tech	19.07.16	IP/Resistivitiy Investigation Along Dornahalli-Madnal Tract, Bhima Basin, A Geophysical Tool for Uranium Exploration
16	Sivakrishna Yavvari (AMD, Hyd.)	M.Tech	19.07.16	Delineation of Suplphide Rich Zones Using IP/Resistivitiy and Magnetic Surveys and Explore the Controlling Factors for Uranijum Mineralization Along Albitite Line, Gumansingh Ki Dhani Area, Rajasthan
17	Togaru Subhash (AMD, Hyd.)	M.Tech	19.07.16	On the Delineation of Structural Features over Pakni-Aniani-JaJawal Sector,Surajpur District, Chhatisgarh, India - An Applkication by Magnetic Method of Geophysical Exploration
18	Hemant Parashar	M.Tech	20.07.16	Separation of U(VI) and Th(IV) from Thorium Concentrate of Monazite Sand using Solvent Extraction Technique
19	Naga Lakshmi Malathi J.	M.Tech	04.08.16	Study and Understanding of Uranium Dioxide Dissolution Behavior in Industrial Plant
20	Vipul Garg	M.Tech	11.08.16	Development of a Framework for Human Reliabillity Assessment via Virtual Simulation
21	Surya Pratap	M.Tech	11.08.16	Performance Evaluation of Compressed IPv6 Payload Over Ysat Network
22	Ashutosh Dwivedi	M.Tech	11.08.16	Development of LabVIEW based GUI to Automate Multiple Sample Positioning Module and to Study the Effect of Slit Size on Positioning accuracy of the Samples at the Scanning EXAFS Beam Line (BL-09), Indus-2 SRS Facility at RRCAT, Indore
23	Shaleen Jain	M.Tech	11.08.16	Study and Design of Algorithm for Active Neutron Interrogation based *llicit Maaterial Detection System*
24	Puneet Kulkarni	M.Tech	11.08.16	Anomalous Packet Identification for Network based Intrusion Detection System
25	Pravin Bhardwaj	M.Tech	12.08.16	Uncertainty Analysis in Using Hall Probe Magnetometers for Qualification of Accelerator
26	Ankur Katiyar	M.Tech	02.09.16	Establishment of Design Margin of Multiply Supported Piping Subjected to High Amplitude denuation Pulse Loads
27	Raman Saini	M.Tech	02.09.16	Investigations to Establish the Conditions to Induce Nodular Corrosion in Zr 2.5% Nb Alloy
28	Paresh Kothari	M.Tech	09.09.16	Effect of Nonlinearity of R.C.C. Structure on the Floor Response Spectra
29	Utpal Bera	M.Tech	29.09.16	Shielding Optimization Studies for a Typical Hot Cell
30	G. Bharat Reddy	M.Tech	10.10.16	Investigation of Effect of Temperature on the Evolution of Texture and Twinning of Zircaloy-4
31	Devarapalli Venkatesh	M.Tech	13.10.16	Design and development of paralleling methodology of Pulse Width Modulated AC to DC converter using phase shifted sinusoidal PWM technique

32	Ravi Mohan	M.Tech	14.10.16	Study on Convective Heat Transfer Behaviour of Spent Fuel Storage Pool in Normal Operating Condition and Station Blackout Condition
33	Roshini Robin	M.Tech	14.10.16	TWO PHASE FLOW VISUALIZATION USING WIRE MESH SENSORS (WMS) IN SUB-CHANNEL MEASURMENTS
34	Anirban Ghosh	M.Tech	14.10.16	Theoretical Modeling and Experimental Validation for Life Assessment of Belleville Spring
35	Rohit Khatri	M.Tech	14.10.16	ESTIMATION OF FATIGUE LIFE OF PLASTIC LEADED CHIP CARRIER (PLCC) SOLDER JOINTS DUE TO VIBRATION AND TEMPERATURE CYCLING
36	Donthula Harish	M.Tech	14.10.16	Understanding Active Eutectoid Phase Transformation in Titanium and Zirconium Alloys
37	Muthukumar S. NFC, Hyd.)	M.Tech	14.10.16	Modeling and Theoretical Analysis of Short Circuit & Inrush Currents for Design & Development of High Temperature Superconducting Transformer
38	Nabiullah Khan	M.Tech	14.10.16	Simulation of Drop Dynamics Behavior in an Extraction Column
39	Manojit Shaw	M.Tech	20.09.16	Characterization of Defects in Austenitic Stainless Steel Tubes by Eddy Current Testing
40	Anita	M.Tech	20.09.16	Use of Raman Tweezers for Analysis of Microbial Cells
41	Amey Lambhate	M.Tech	18.10.16	Equipment-structure inteaction due to secondary waves generated by underwater explosions
42	Sparsh Kumar Sharma	M.Tech	21.10.16	Development of simulator model of Dhruva for real time closed loop simulation testing of RRS
43	Swagata Chatterjee	M.Tech	21.10.16	A MODEL BASED APPROACH FOR FAULT DETECTION AND DIAGNOSIS OF THREE PHASE INDUCTION MOTOR
44	Abhishek Kumar Singh	M.Tech	30.11.16	Cyclic and shakedown assessment of thick vessels (cylinders) with openings subjected to pressure and thermal cycles
45	Shalini N	M.Tech	30.11.16	Design of a Waveguide for a Radar Based Level Instrument & Formulation of Appropriate Signal Processing Techniques for Improving Accuracy of Interface Level Measurment in a Joule Melter
46	Saumya Upadhyay (NFC, Hyd.)	M.Tech	30.11.16	NUMERICAL SIMULATION AND EXPERIMENTAL STUDY OF EFFECT OF DIE PROFILE ON HOT EXTRUSION OF ZIRCALOY-4
47	Bikram Kumar	M.Tech	26.12.16	
48	Uday Kumar Vootla	M.Tech	29.12.16	IMPROVING THE PERFORMANCE OF VENTURI SCRUBBER FOR HF ABSORPTION
49	Pratik Bhardwaj	M.Tech	14.10.16	DESIGN AND ANALYSIS OF FUEL PIN MAGAZINE HOLDER UNDER ACCIDENTAL CONDITION

50	Kolhatkar Ashish Vallabh	M.Tech	14.10.16	DEVELOPMENT AND VALIDATION OF ULTRA SUBSIZE TENSILE SPECIMEN
51	Katra Sandeep (NFC, Hyderabad)	M.Tech	29.12.16	Optimization study in Distillation columns for improved performance by approaching ideal cascade
52	Sajja Suresh	M.Tech	04.01.17	Analysis and design of Single Spoke Resonators (SSR) for acceleration of protons and heavy ions
53	Mahima Shukla	M.Tech	04.01.17	Multi-Scale Detection of Seismic Phases on Three Component Broad Band Seismic Records
54	Vipin A. S.	M.Tech	21.10.16	DESIGN AND ANALYSIS OF REMOTELY OPERABLE HIGH TEMPERATURE PIPELINE CONNECTOR
55	Deepak N Mathad	M.Tech	04.01.17	DESIGN AND ANALYSIS OF TRANSVERSE BEAM EMITTANCE MEASUREMENT SYSTEM USING SLIT GRIDTECHNIQUE
56	Shahnawaz Ahmad	M.Tech	04.01.17	Effect of residual stresses on fatigue crack growth behaviour of dissimilar metal pipe weld joints: SA508 and SS304LN
57	Subrata Dey	M.Tech	04.01.17	To study the effect of a/W and strain hardening exponent (n) on h factor for TPB specimen and throughwall circumferentially cracked straight pipe subjected to bending moment loading
58	Madhusudan Sharma	M.Tech	10.01.17	DESIGN, DEVELOPMENT AND MAGNETIC TESTING OF PROTOTYPE DISC TYPE OF HALBACH ARRAY BASED PERMANENT MAGNET ELECTROMAGNETIC PUMP
59	Sushant Sarswat	M.Tech	9.02.17	Comparative Evaluation of Processing Techniques for Management of Low Level Radioactive Liquid Wastes
60	Shobhna Mishra	M.Tech	25.11.16	Electromagnetic expansion welding studies of Aluminium 6061 tube to Aluminium 6061 flange with 40 kJ capacitor bank
61	Pankaj Kumar Battabyal (NFC,Hydrabad)	M.Tech	27.02.17	Study and Optimization of Process Parameters of Degreasing of Zircaloy Tubes
62	Anik Das	M.Tech	08.03.17	Synthesis of U-0.6 wt.%Ti and study of its Aging behaviour
63	Uttam Kumar Sahoo (NFC,Hydrabad)	M.Tech	09.03.17	Mathematical Modelling and Simulation Studies on Vacuum Distillation Cascade for Optimization of Operating Parameters
64	Shyam Sunder Mahto (NFC,Hydrabad)	M.Tech	09.03.17	Analysis of Radial Flow Ammonia Synthesis Reactor
65	Meenakshi Mehra	M.Tech	22.03.17	Thermal hydraulic design of intermediate heat exchanger for commercoal fast breeder reactor
66	Snehal Dattatraya Ghule	M.Tech	22.03.17	Recombination of hydrogen, produced in the cover gas of a nuclear reactor with oxygen in presence of Palladium catalyst
67	Ashok Kumar	M.Tech	22.12.16	Performance testing of high speed centrifuge
68	Aswin Pradeep	M.Tech	22.12.16	Solvent Extraction Studies on Alkali Leached Specific Sodium Di-uranate Feed

69	Sanam Khan	M.Tech	23.12.16	Online Condition Monitoring System using Wireless Sensor Network
70	Garima Singal	M.Tech	22.08.16	Study on the Start-Up Behavior of a Natural Circulation Pressure Tube Type BWR-Experimental and Numerical Simulations
71	Aman Agarwal (NFC., Hyd.)	M.Tech	22.08.16	Experiment nad FE Analysis of Double -Arc Shaped Non-Standard Curved Compact Tension Specimens for Study of Fracture Behaviour of Zircaloy-4 Fuel-Clad Tubes
72	Wahdat Safia	M.Tech	22.08.16	Study and Development of Heuristic-based Algorithm for Virtual Machine Placement in Cloud Computing Environment
73	Udai Giri Pratap Singh Sachan	M.Tech	29.12.16	2D-Quench Analysis of Superconducting Solenoid Magnet by using Numerical Methods
74	Siva Rama Krishna B	M.Tech	29.12.16	Development of base isolation technique for controlling the response of the ical detector subjected to earthquake, transient magnetic forces and ground shock independently
75	Mohammad Afaash	M.Tech	22.08.16	Design of RF Reference Phase Distrubution System
76	Vinod Kumar	M.Tech	22.08.16	Development of pressure vessel using probabilistic fracture mechanics
77	Sumit Raghuvanshi (NFC., Hyd.)	M.Tech	22.08.16	Comparative study of high temperature design of pellet carrier boat using various materials
78	Nancy Semwal	M.Tech	22.08.16	Change detection in satellite images
79	Ather Syed	M.Tech	31.08.16	Model Development for pressure tube deformation of Indian PHWRs under symmetric and asymmetric heat up condition
80	Robin Bhola	M.Tech	31.08.16	Assessment of Ultimate Lpoad Capacity (ULC) of LWR steel lined inner containment (IC) structure
81	Shaikh Aatef Kamal	M.Tech	31.08.16	Studies on the use of cmos active pixel sensor in radiation monitoring
82	Samadrita Chakraborty	M.Tech	09.01.17	Study of characteristics and comparative performance of film and digital radiography techniques
83	Neha Rani Yadav	M.Tech	27.10.16	Development/Real Time Implementation of Singnal Estimation and Dynamic Compensation Algorithm for Delayed Self Powered Neutron Detectors
84	Tummalapalli Naga Srinivas	M.Tech	27.10.16	Study of frequency dependence of response of block type machine foundations
85	Zahoor Ahmed Dar	M.Tech	27.10.16	"Analytical study and design of high current, high power repetitive capacitor charging power supply"
86	Sudeshna Saha	M.Tech	1.12.16	Hybrid adsorbents for the removal of U, Th and Cs from aquatic medium
87	Saparya Chattaraj	M.Tech	1.12.16	Assessment of Pyrophoric Behavior of Uranium Flakes for Safe Storage and Handling
88	Jayant Krishan	M.Tech	1.12.16	Development of a parallel program to compute external doses from a radioactive cloud

89	Anisha Acharya	M.Tech	29.12.16	Development of Mathematical Model and Signal Analysis Algorithm for Fabry Perot Interferometer based Vibration Measurement
90	Purva Dhawan	M.Tech	09.03.17	Computational fluid dynamics based steam condensation modeling in the presence of non-condensable gases for containment thermal hydraulics
91	Divya Shukla	M.Tech	29.12.16	Design, simulation & prototype development of solid state, IGBT based, PWM controlled, SMPS for heating of simulated nuclear fuel cluster for Nuclear Power Plants
92	Premananda Dey	M.Tech	20.01.17	Design and development of optically isolated electrical measurementand voltage measurement
93	Shyam Sundar Jena	M.Tech	20.01.17	Study of different power dividers/ combiners and design & development of planer gysel type power divider for solid state radio frequency power amplifier for accelerator application
94	Kallol Mukherjee	M.Tech	20.01.17	Optimization of conjugate heat transfer in an electron beam dump
95	Debangana Sarkar	M.Tech	31.03.17	Design of an efficient data storage architecture for large unstructured data
96	Prateek Kumar Laxminarayan Mishra	M.Tech	04.04.17	Hydrodynamic and Chemical Studies of Neodymium extraction using Pseudo-emulsion Hollow Fiber Liquid Member

S. No.	Name	Degree	DOAPD	Thesis Title
1	Praveen K.	M.Sc.(Engg.)	14.09.16	Design and Development of Novel Liquid Level Sensor and its Wireless Measurement System
2	Sushil Kumar	M.Sc.(Engg.)	13.12.16	“Development of H_2S Sensors for Industrial Applications”
3	Parshuram Yedba Bhosale	M.Sc.(Engg.)	22.12.16	Development of Human Factors in Support of Safety Analysis in Nuclear Plant
4	Sarvajit Kumar	M.Sc.(Engg.)	22.12.16	Development of Variable Frequency Damper for Controlling Vibration and Seismic Response for Piping System
5	Chandra Bahadur	M.Sc.(Engg.)	26.12.16	Design and Development of Time to Count Technique to eliminate dead time and saturation effects of Conventional GM
6	Santosh M. Raut	M.Sc.(Engg.)	26.12.16	Time Stamped Pulse Acquisition Technique for Nuclear Physics and other Research Experiments
7	Lalit Mohan	M. Sc. (Engg.)	22.03.17	Workspace Characterization and Error Modelling of 5-DOF Hybrid Manipulator
8	Chandrajeet Yadav	M. Sc. (Engg.)	22.03.17	Cfd modelling of scaled-up hydrogen-fluorine flame reactor

Section –V

List of completed D.M.,M.Ch. and M.D. dissertations during 2016-17

List of D.M./M.Ch./M.D. Dissertations for which results were notified during April 1,2016 to March 31,2017

S. No.	Name	CI	Degree	DOAPD
1	Bhosale Shilpushp Jagannath	TMC	DM-Critcal Care	28.07.16
2	Rakesh Pinninti	TMC	DM-Med.Onclgy	28.07.16
3	Sunny Jandyal	TMC	DM-Med.Onclgy	28.07.16
4	Naga Avinash Bonda	TMC	DM-Med.Onclgy	28.07.16
5	Chandrakanth M.	TMC	DM-Med.Onclgy	28.07.16
6	Vivek Agarwala	TMC	DM-Med.Onclgy	28.07.16
7	Sanyo P. Dsouza	TMC	DM-Med.Onclgy	28.07.16
8	Mansi Sharma	TMC	DM-Med.Onclgy	28.07.16
9	Davinder Paul	TMC	DM-Med.Onclgy	28.07.16
10	Shruti Kate	TMC	DM-Med.Onclgy	28.07.16
11	Zanwar Saurabh	TMC	DM-Med.Onclgy	28.07.16
12	Sachin Khurana	TMC	DM-Med.Onclgy	28.07.16
13	Abraham Samuel	TMC	DM-Med.Onclgy	28.07.16
14	Suhail Sarwar Siddiqui	TMC	DM-Critcal Care	28.07.16
15	Natesh Prabhu R.	TMC	DM-Critcal Care	28.07.16
16	Jasmeet Singh Dhingra	TMC	DM-Gastro	28.07.16
17	Virpariya Mukundkumar Mansukhlal	TMC	DM-Gastro	28.07.16
18	Sneha Tandon	TMC	DM-Pad.Onclgy	28.07.16
19	Nirmalaya Deo Pradhan	TMC	DM-Pad.Onclgy	28.07.16
20	Deepak Shashikant M.	TMC	DM-Med.Onclgy	03.01.17
21	Arif Mohammed Khan S.	TMC	DM-Med.Onclgy	03.01.17

S. No.	Name	CI	Degree	DOAPD
1	Neha Kumar	TMC	MCh.- G.Ocly	28.07.16
2	Amruta Nikhil Beke	TMC	MCh.- S.Ocly.	28.07.16
3	Pavan T. Sugoor	TMC	MCh.- S.Ocly.	28.07.16
4	Vijayraj S. Patil	TMC	MCh.- S.Ocly.	28.07.16
5	Ghose Joy	TMC	MCh.- S.Ocly.	28.07.16
6	Ingle Parag Ramesh	TMC	MCh.- S.Ocly.	28.07.16
7	Jiwnani Sabita Shambhulal	TMC	MCh.- S.Ocly.	28.07.16
8	Naveena Kumar A.N.	TMC	MCh.- S.Ocly.	28.07.16
9	Kamlesh Verma	TMC	MCh.- S.Ocly.	28.07.16
10	Sunil Navalgund	TMC	MCh.- S.Ocly.	28.07.16
11	Shah Sanket Bharat	TMC	MCh.- S.Ocly.	28.07.16
12	Shinde Rajesh Sitaram	TMC	MCh.- S.Ocly.	28.07.16
13	Nizamudheen M.P.	TMC	MCh.- S.Ocly.	28.07.16
14	Anam Jay Rashmi	TMC	MCh.- S.Ocly.	28.07.16
15	Bharath G.	TMC	MCh.- S.Ocly.	28.07.16
16	Richa Vaish	TMC	MCh-Hd&Neck Surg	28.07.16
17	Swagnik Chakrabarti	TMC	MCh-Hd&Neck Surg	28.07.16

18	Bhujbal Vidisha Sachin	TMC	MCh-Hd&Neck Surg	28.07.16
19	Shilpi Sharma	TMC	MCh-Hd&Neck Surg	28.07.16
20	Rajendr Dilip Dhondge	TMC	MCh.-Plastic & Reconstructive Surgery	28.07.16
21	Saumya Mathews	TMC	MCh.-Plastic & Reconstructive Surgery	28.07.16
22	Gaurav Khandelwal	TMC	MCh.- S.Ocly.	03.01.17
23	Verma Harish Suganraj	TMC	MCh.- S.Ocly.	03.01.17

S. No.	Name	CI	Degree	DOAPD
1	Subhashreddy Doni	TMC	MD-Rad.Diagn	17.08.16
2	Doshi Nidhi Mahendra	TMC	MD-Rad.Diagn	17.08.16
3	Dengale Kalyani Vinayak	TMC	MD-Rad.Diagn	17.08.16
4	Asore Machindranath Tukaram	TMC	MD-Rad.Diagn	17.08.16
5	Santhosh Kumar G.V.	TMC	MD-Rad.Diagn	17.08.16
6	Shinde Vikas Ganesh	TMC	MD-Rad.Diagn	17.08.16
7	Gite Prashant Murlidharrao	TMC	MD-Rad.Diagn	17.08.16
8	Patil Utkarsh Chandrakant	TMC	MD-Rad.Diagn	17.08.16
9	Somesh Singh	TMC	MD-Rad.Diagn	17.08.16
10	Suresh Kumar G.	TMC	MD-Rad.Diagn	17.08.16
11	Jain Nikshita Akshay	TMC	MD-Rad.Diagn	17.08.16
12	Amit Yadav	TMC	MD-Anaesly.	17.08.16
13	Patil Sanika Jayant	TMC	MD-Anaesly.	17.08.16
14	Menon Deepika Harish	TMC	MD-Anaesly.	17.08.16
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48	Maitre Madan Prakash	TMC	MD-Rad.Thy.	17.08.16
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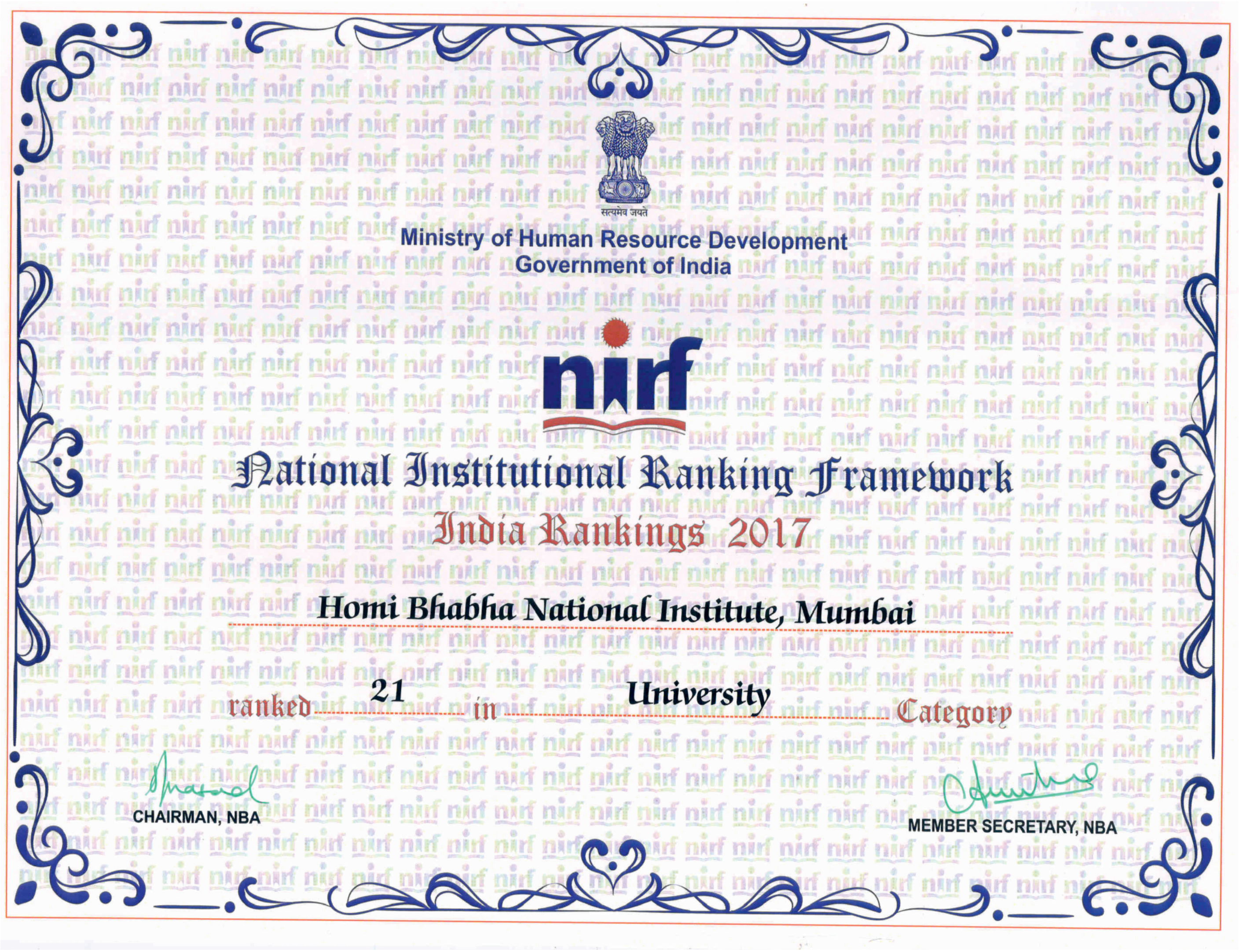
63	Raghavindra K.	TMC	MD-Anaesly.	03.01.17



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Ministry of Human Resource Development
Government of India

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National Institutional Ranking Framework

India Rankings 2017

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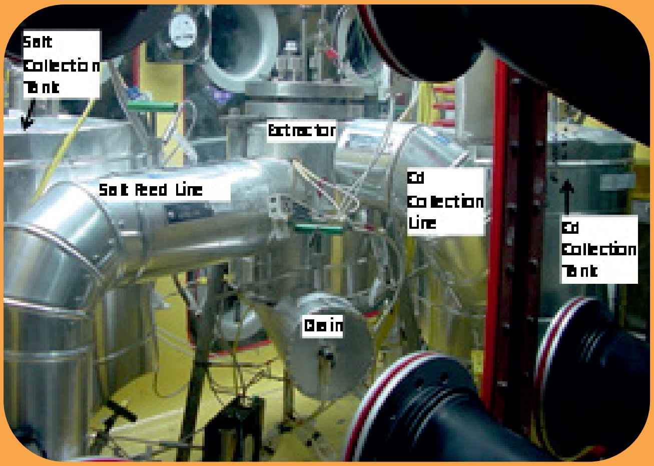
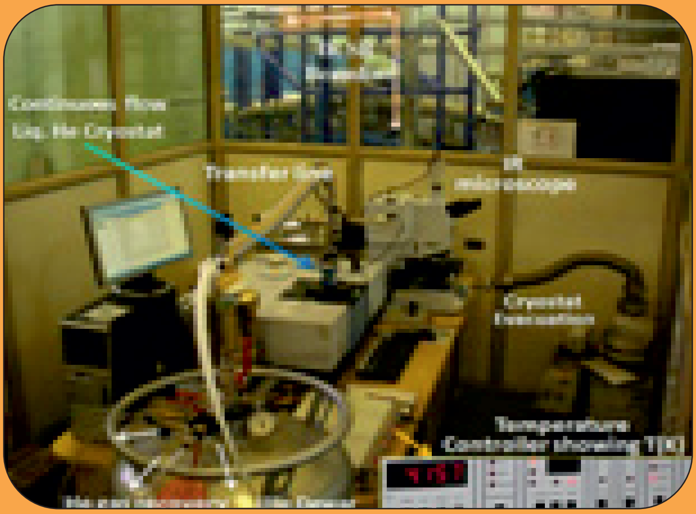
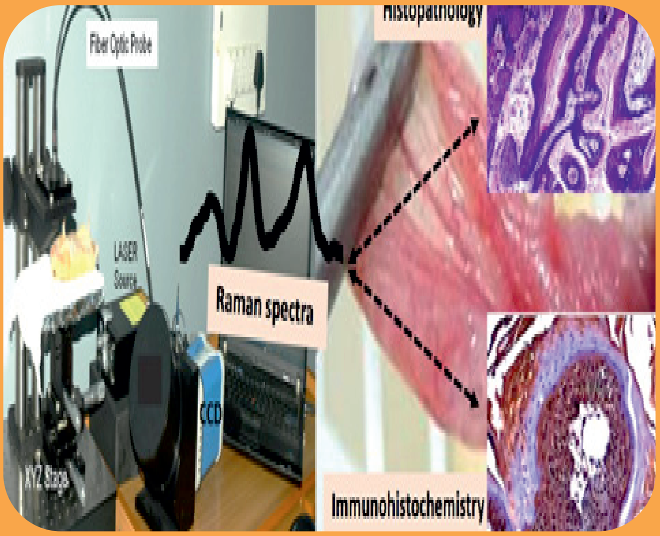
Dilution refrigerator set-up



High temperature molten salt extraction setup with heaters



Infra-red beam line sample station



Raman spectroscopy in experimental oral carcinogenesis

होमी भाभा राष्ट्रीय संस्थान

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