होमी भाभा राष्ट्रीय संस्थान

Homi Bhabha National Institute

Bhabha Atomic Reserch Centre

Indira Gandhi Centre for Atomic Research

Raja Ramanna Centre for Advanced Technology

Variable Energy Cyclotron Centre

Saha Institute of Nuclear Physics

Institute for Plasma Research

Institute of Physics

Harish-Chandra Research Institute

Tata Memorial Centre

Institute of Mathematical Sciences

ANNUAL REPORT

2012- 2013

(Volume-2)

**Training School Complex
Bhabha Atomic Research Centre
Anushaktinagar, Mumbai 400 094**

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Front cover page : Photographs of the 10 Constituent Institutions of HBNI

Annex 1

Composition of the Bodies of the Institute

Council of Management
(CoM)

Prof. S. Banerjee	Chairman (up to 30.04.2012)
Dr. Ratan Kumar Sinha Chairman, AEC	Member up to 30.04.2012 Chairman (w.e.f 01.05.2012)
Prof. R.B. Grover Director HBNI	Member
Shri V. V. Bhat Member for Finance, AEC	Member
Shri Ashok Thakur Secretary Higher Education, MHRDD	Member
Prof. Arun Nigavekar Trustee & Senior Advisor, Science & Technology Park, University of Pune	Member
Prof.Sudhir K. Sopory Vice-Chancellor Jawaharlal Nehru Unversity New Delhi	Member
Shri S.C. Chetal	Member (upto 31.01.2013)
Prof. P.R. Vasudeva Rao Director, IGCAR	Member (w.e.f. 01.02.2013)
Prof. R.A. Badwe Director, TMC	Member
Prof. P.K. Kaw	Member (upto 31.01.2013)
Prof. Dhiraj Bora Director, IPR	Member (w.e.f. 01.02.2013)
Shri S. Basu Director, BARC	Member (w.e.f. 18.09.2012)
Prof R R Puri	Member-Secretary (up to 30.11.2012)
Prof. B. K. Dutta Dean HBNI	Member-Secretary (w.e.f. 01.12.2012)

Academic Council

Prof. R.B. Grover	Chairman
Prof. S.K. Apte	Convener, Board of Studies in Life Sciences
Prof. R. Ramanujam	Convener, BoS Mathematical Sciences
Prof.. R. A. Badwe	Director, TMC
Prof. R. Balasubramanian	Director, IMSc
Shri S.C. Chetal / Prof. P.R. Vasudeva Rao	Director, IGCAR
Prof. Dinesh Srivastava	Director, VECC
Prof. B.M.Deb	IISER, Kolkata
Prof. P.K. Vijayan	Convener, Board of Studies in Engineering Sciences
Prof. Dipan Ghosh	IIT-Bombay
Prof. P.D.Gupta	Director, RRCAT
Prof. Jayanta K. Bhattacharjee	Director, HRI
Prof. P.K. Kaw / Prof. D. Bora	Director, IPR
Prof. A.M. Jayannabar	Director, IoP
Prof. K. Muralidhar	IIT-Kanpur
Prof. Srinivasa Ranganathan	IISc, Banglore
Prof. S.Ramakrishnan	TIFR, Mumbai
Prof. K.L. Ramakumar	Convener, Board of Strategic Studies
Prof. M.K. Sanyal	Director, SINP
Shri S. Basu	Director, BARC
Dr. K. S. Sharma	Convener, BoS, Health Science, TMC
Prof. Dinesh Srivastava	Convener, BoS Physical Sciences
Prof. R.R. Puri/ B.K. Dutta	Member Secretary

Advisory Committee

Prof. S. Banerjee / Dr. R.K. Sinha, Chairman, AEC	Chairman
Prof. R.A.Badwe Director, TMC	Member
Prof. R. Balasubramanian Director, IMSc	Member
Shri S.C Chetal / Prof. P.R. Vasudeva Rao , Director, IGCAR	Member
Prof. M. Barma Director, TIFR	Member
Prof. T.K. Chandrashekar Director, NISER	Member
Prof. R.B. Grover Director, HBNI	Member
Prof. Jayanta K. Bhattacharjee Director, HRI	Member
Prof. P.K. Kaw / Prof. D. Bora, Director, IPR	Member
Prof. P.D.Gupta Director, RRCAT	Member
Prof. Dinesh Srivastava Director, VECC	Member
Prof. M.K.Sanyal Director, SINP	Member
Shri S. Basu Director, BARC	Member
Prof. A.M.Jayannabar Director, IoP	Member
Prof. R.R. Puri/ B.K. Dutta Dean, HBNI	Member-Secretary

Board of Studies of HBNI

Physical Sciences

1. Prof. Dinesh Srivastava   **Convener**
    Variable Energy Cyclotron Centre

2. Prof. C.S.Sundar
    Indira Gandhi Centre for Atomic Research

3. Prof. S Ganesh
    Institute of Plasma Research

4. Prof. Ajit Srivastava
    Institute of Physics

5. Prof. P.K.Gupta
    Raja Ramanna Centre for Advanced Technology

6. Prof. Pinaki Majumdar
    Harish-Chandra Research Institute

7. Prof. P. Mitra
    Saha Institute of Nuclear Physics

8. Prof.Ghanashyam Date
    Institute of Mathematical Sciences

9. Prof. B.N.Jagtap
    Bhabha Atomic Research Centre

10. Prof. S L Chaplot
    Bhabha Atomic Research Centre

Chemical Sciences

1. Prof. K.L. Ramakumar   **Convener**
    Bhabha Atomic Research Centre

2. Prof.A.V.R. Reddy
    Bhabha Atomic Research Centre

3. Prof. A. Goswami
    Bhabha Atomic Research Centre

4. Prof. Swapan Ghosh
    Bhabha Atomic Research Centre

5. Prof. V. Ganesan
    Indira Gandhi Centre for Atomic Research

6. Prof. K. Nagarajan
    Indira Gandhi Centre for Atomic Research

7.   Prof. V.K Jain
    Bhabha Atomic Research Centre

8. Prof. A. Srinivasan
    Head, School of Chemistry, NISER (IOP)

9. Prof. S. Chattopadhyaya
    Bhabha Atomic Research Centre

Life Sciences

1. Prof. S.K. Apte   **Convener**
   Bhabha Atomic Research Centre

2. Prof. (Mrs.) S. Chiplunkar
   Advanced Centre for Treatment, Research
   & Education in Cancer (ACTREC)

3. Prof. Rita Mulherkar
   Advanced Centre for Treatment, Research
   & Education in Cancer (ACTREC)

4. Prof. S. P Kale
   Bhabha Atomic Research Centre

5. Prof. J.R. Bandekar
   Bhabha Atomic Research Centre

6. Prof. A.K.Sharma
   Bhabha Atomic Research Centre

7. Prof. B.J.Rao
   Tata Institute of Fundamental Research

8. Prof. Dipak Dasgupta
   SINP

Engineering Sciences

1. Prof. P.K. Vijayan   **Convener**
   Bhabha Atomic Research Centre

2. Prof. G. K. Dey
   Bhabha Atomic Research Centre

3. Prof. Hubli
   Bhabha Atomic Research Centre

4. Prof. T.Jayakumar
   Indira Gandhi Centre for Atomic Research

5. Prof. B. K. Dutta
   Bhabha Atomic Research Centre

6. Prof. A. P. Tiwari
   Bhabha Atomic Research Centre

7. Prof. Kamachi Mudali
   Indira Gandhi Centre for Atomic Research

8. Prof. Kallol Roy
   Bhabha Atomic Research Centre

9. Prof. P. V. Varde
   Bhabha Atomic Research Centre

10. Prof. D. N. Badodkar
    Bhabha Atomic Research Centre

Mathematical Sciences

1. Prof. R. Ramanujam   **Convener**
   Institute of Mathematical Sciences

2. Prof. Amritanshu Prasad
   Institute of Mathematical Sciences

3. Prof. B. Ramakrishnan
   Harish-Chandra Research Institute

4. Prof. V.S.Sunder
   Institute of Mathematical Sciences

5. Prof. N. Raghavendra
   Harish-Chandra Research Institute

6. Prof. R.C.Cowsik
   Mumbai University

7. Prof. Murali Srinivasan
   Indian Institute of Technology-Bombay

8. Prof. Madhavan Mukund
   Chennai Mathematics Institute

9. Prof. Muruganandam
   NISER

Strategic Studies

1. Prof. K.L. Ramakumar   **Convener**
   Bhabha Atomic Research Centre

2. Dr. A.K. Kohli
   Board of Radiation and Isotope Technology

3. Prof. R. B. Grover
   Director HBNI

4. Dr. B.B. Singh
   Ex-BARC and Scientific Advisor, High Court, Mumbai

5. Prof. Rangan Banerjee
   Indian Institute of Technology-Bombay

6. Prof. M. Sai Baba
   Indira Gandhi Centre for Atomic Research

7. Dr. J Kumar
   Legal Adviser, DAE

Board of Health Sciences

1. Prof. K. S. Sharma   **Convener**
   Tata Memorial Centre, Mumbai

2. Prof. D D Deshpande
   Tata Memorial Hospital, Mumbai

3.   Prof. K. B. Sainis
       Bhabha Atomic Research Centre, Mumbai

4.   Prof. S. K. Srivastava
       Tata Memorial Hospital, Mumbai

5.   Dr. H.B.Tongaonkar
       Tata Memorial Hospital, Mumbai

6.   Dr S.B.Banavali
       Tata Memorial Hospital

7.   Prof. N. A. Jambekar
       Tata Memorial Hospital, Mumbai

8.   Prof. Shubhangi Parkar
       KEM Hospital, Mumbai

9.   Prof. Avinash Supe
       LTMG Hospital, Mumbai

10.   Prof. M.G.R. Rajan
       Radiation Medicine Centre, Mumbai

Officers of the Institute

Academic

Prof. R.B. Grover	Director
Prof. R.R. Puri/ Prof. B.K. Dutta	Dean
Dr. R.P. Patel	Associate Dean

Administrative and Accounts

Shri A. Ramaiah	Finance Officer
Ms B. Lata	Administrative Officer
Shri Yellapan	Accounts Officer

Deans-Academic at the CIs

BARC

Prof. S.K. Apte	Life Sciences (Coordinating Dean at BARC for HBNI)
Prof. B.K.Dutta/ G.K. Dey	Engineering Sciences
Prof. B.N. Jagatap	Physical Sciences
Prof. Swapan K. Ghosh	Chemical Sciences

IGCAR

Prof. V. Ganesan   Chemical Sciences

Prof. B.V.R. Tata   Physical Sciences

Prof. T. Jayakumar   Engineering Science

RRCAT

Prof. S.B.Roy

VECC

Prof. Jane Alam   Physical Sciences

Prof. D. Sarkar   Engineering Science

SINP

Prof. P. Mitra

IPR

Prof. S Mukherjee

IoP

Prof. Ajit Srivastava

NISER - IoP

Prof. Varadharajan Muruganandam

TMC

Prof. K.S.Sharma

IMSc

Prof. Vijay Kodiyalam   Mathematical Science

Prof. Ghanashyam Date   Physical Sciences

HRI

Prof. Pinaki Majumdar

Annex 2

Standing Committees

BARC Standing Committees

Physical Sciences

1. Dr. S. Kailas — Chairman
2. Dr. Amber Chatterjee — Member
3. Dr. S.L. Chaplot — Member
4. Dr. S.V.G. Menon — Member
5. Dr. S.M. Sharma — Member
6. Dr. Amar Sinha — Member
7. Dr. K.C. Mittal — Member
8. Dr. N.K. Sahoo — Member
9. Dr. P.D. Krishnani — Member
10. Dr. D.N. Sharma — Member
11. Dr. A.K. Das — Member
12. Dr. Satish Gupta — Member
13. Dr. B.N. Jagatap — Convener

Chemical Sciences

1. Dr. T. Mukherjee — Chairman (upto 31.12.12)
2. Dr. K.L. Ramakumar — Chairman (w.e.f. 01.01.13)
3. Dr. D. Das — Member
4. Dr. S.K. Sarkar — Member
5. Dr. A V R Reddy — Member
6. Dr. J. Arunachalam — Member
7. Dr. M. R. A. Pillai — Member
8. Dr. A. K. Goswami — Member
9. Dr. B. S. Tomar — Member
10. Dr. S.K. Aggarwal — Member
11. Dr. L. Vashney — Member
12. Dr. S. Chattopadhyay — Member
13. Dr. S.K. Ghosh — Convener

Life Sciences

1. Dr. K.B. Sainis — Chairman
2. Dr. S.F. D'Souza — Member
3. Dr. M. Seshadri — Member
4. Dr. A.K. Sharma — Member
5. Dr. M.G.R. Rajan — Member
6. Dr. M.V. Hosur — Member
7. Dr. S.K. Apte — Convener

Engineering Sciences & Strategic Studies

1.	Dr. A.K. Suri	Chairman
2.	Dr. L.M. Gantayet	Member
3.	Dr. R.K. Singh	Member
4.	Dr. P.K. Vijayan	Member
5.	Dr. A.P. Tiwari	Member
6.	Dr. M.S. Bhatia	Member
7.	Dr. P. Varde	Member
8.	Dr. D. Sathiyamoorthy	Member
9.	Dr. V.K. Suri	Member
10.	Dr. B.K. Dutta	Convener

RRCAT Standing Committee

1.	Dr. P.D. Gupta	Chairman
2.	Dr. P.K. Gupta	Member
3.	Dr. L.M. Kukreja	Member
4.	Shri C.P. Navathe	Member
5.	Dr. G.S. Lodha	Member
6.	Dr. P.A.Naik	Member
7.	Dr. S.K.Deb	Member
8.	Dr. S.M.Oak	Member
9.	Shri P.R.Hannurkar	Member
10.	Dr. Arup Banerjee	Member
11.	Dr. A. Chowdhury	Member
12.	Dr. S.B. Roy	Dr. S.B. Roy

IGCAR Standing Committees

Physical Sciences

1.	Dr. C.S. Sundar	Chairman
2.	Dr. A. K. Arora	member
3.	Dr. M.Vijialakshmi	Member
4.	Dr. B.Venkatraman	Member
5.	Dr. K. G. M. Nair	Member
6.	Dr. A.K. Tyagi	Member
7.	Dr. B.V.R. Tata	Member
8.	Dr. John Philip	Member
9.	Dr. N. Subramanian	Member
10.	Dr. R.S.Keshavamurthy	Member
11.	Dr. M. Sai Baba	Member
12.	Dr. G. Amarendra	Convener

Chemical Sciences

1.	Dr. K. Nagarajan	Chairman
2.	Dr. V. Ganesan	Member
3.	Dr. U. Kamachi Mudali	Member
4.	Dr. S. Anthonysamy	Member
5.	Dr. A. Bharathi	Member
6.	Dr. N. Sivaraman	Member
7.	Dr. C. Mallika	Member
8.	Dr. V. Jayaraman	Member
9.	Dr. M. Sai Baba	Member
10.	Dr. K.V.G. Kutty	Convener

Engineering Sciences

1.	Dr. T. Jayakumar	Chairman
2.	Dr. P. Chellapandi	Member
3.	Dr. S. Venugopal	Member
4.	Dr. A.K. Bhaduri	Member
5.	Dr. U. Kamachi Mudali	Member
6.	Dr. C. Anand Babu	Member
7.	Dr. K. Velusami	Member
8.	Dr. B.P.C. Rao	Member
9.	Dr. B.K. Panigrahi	Member
10.	Dr. Saroja Sai Baba	Member
11.	Dr. K.Nagarajan	Member
12.	Dr. G. Sasikala	Member
13.	Dr. M. Sai Baba	Convener

VECC Standing Committee

1.	Dr. D.K. Srivastava	
2.	Dr. Alok Chakrabarti	
3.	Dr. Y.P. Viyogi	
4.	Shri Subimal Saha	
5.	Dr. D Sarkar	(Convener, Engineering Sciences)
6.	Dr. Saila Bhattacharya	
7.	Shri Gautam Pal	
8.	Dr. S. R. Banerjee	
9.	Dr. A.K. Chaudhuri	
10.	Dr. P. Barat	
11.	Dr. V.S. Pandit	
12.	Dr. Jane Alam	(Convener, Physical Sciences)
13.	Dr. Subhasis Chattopadhyay	
14.	Dr. Tapan Kumar Nayak	
15.	Dr. (Smt.) Paramita Mukherjee	

IPR Standing Committee

1.	Prof S Mukherjee	Chairman
2.	Prof S Sengupta	Member
3.	Dr D Raju	Member
4.	Dr R Srinivasan	Member
5.	Dr M Bandyopadhyay	Member
6.	Dr PK Atrey	Member
7.	Dr A Srivastava	Member

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Annex 3

Faculty List (01 April 2012 to 31 March 2013)

BARC

Chemical Sciences

1. Achary S.N.
2. Acharya R.
3. Achuthan P.V. Adhikari S.
4. Agarwal Renu (Ms.)
5. Aggarwal S.K.
6. Ali S.K. Musharaf
7. Anshu Singhal (Ms.)
8. Arunachalam J.
9. Arya Ashok Kumar
10. Aswal D.K.
11. Awadhesh Kumar
12. Bajaj P.N.
13. Bandyopadhyay Tusar
14. Banerjee A. (Ms.)
15. Banerjee Sharmila (Ms.)
16. Bharadwaj Mrs). S.R.
17. Bharadwaj Y.K.
18. Bhasikuttan A.C.
19. Bindal R.C.
20. Chattopadhyay A.
21. Chattopadhyay Subrata
22. Chaudhury Niharendu
23. Chaurasia Sheo Chandra
24. Chowdhury D.P.
25. Das D.
26. Das Tapas
27. Das Tomi Nath
28. Dash Ashutosh
29. Deo Mukul Narayan
30. Dey Ghasiram
31. Dhanya S.
32. Dutt G.B.
33. Ganguly R.
34. Gauri G. Pandit (Ms.)
35. Ghanty Tapan Kumar
36. Ghosh Asim Kumar
37. Ghosh Hirendra Nath
38. Ghosh S.K.
39. Ghosh S.K.
40. Ghosh Swapan
41. Goswami Madhumita (Ms.)
42. Goswami A.
43. Hassan P.A.
44. Indira Priyadarsini (Ms.) K.
45. Jai Kumar Sunil
46. Jain V.K.
47. Jha S.K.
48. Kadam R.M.
49. Kalsi Puran Chand
50. Kannan S.
51. Kapoor Sudhir
52. Kaushik C.P.
53. Kayasth S.R.
54. Krishnamurthy Nagaiyar
55. Kshirsagar R.J.
56. Kulshreshtha S.K.
57. Kumar Sangita D. (Ms.)
58. Maity Dilip Kumar
59. Majumder C.
60. Manchanda V.K.
61. Manmohan Kumar
62. Meera Venkatesh (Mrs.)
63. Mishra N.L.
64. Mishra R.
65. Mohanty . Jyoti (Ms.)
66. Mohapatra Prasanta Kumar
67. Mukerjee S.K.
68. Mukherjee Tulsi
69. Murali M.S.
70. Naik Y.P.
71. Naik Devidas B.
72. Naik Prakash Dattatray
73. Natarajan V.
74. Nayak A.K.
75. Nayak Sandip Kumar
76. Padmanabhan P.V.A.
77. Pal Haridas
78. Palit Dipak Kumar
79. Pandey A.K.
80. Parida S.C.
81. Parthsarathy Venkatachari
82. Pathak P.N.
83. Patra Chandra Nath
84. Pillai M.R.A.
85. Pujari Pradeep Kumar
86. Ramachandran V.
87. Ramakumar K.L.
88. Ramamoorthy N.
89. Ramkumar Jayashree (Ms.)
90. Ravi P.M.
91. Ray A.K.
92. Reddy A.V. R.

93. Sabharwal Sunil
94. Sali S.K.
95. Samanta Alok Kumar
96. Samanta S.K.
97. Sarkar S.K.
98. Sasikala Ms. R.
99. Sawant Ramesh Mahadeo
100. Sharma Anubha
101. Shashikala K.
102. Shivanna K.
103. Singh Ajay K.
104. Singh Dhruva Kumar
105. Singhal Rakesh Kumar
106. Sivan Pillai C.G.
107. Smruti Dash (Ms.)
108. Sudarsan V.
109. Sukhendu Nath
110. Tomar B.S.
111. Tripathi A.K.
112. Tripathi R.M.
113. Tyagi A.K.
114. Varshney Lalit
115. Vatsa R.K.
116. Venkataramani B.
117. Venkateswaran G.
118. Venugopal V.
119. Verma Rakesh
120. Yakhmi J.V.

Engineering Sciences

1. Awasthi Alok
2. Badodkar D.N.
3. Balasubramaniam R.
4. Bhargava Kapilesh
5. Bhatia M.S.
6. Bhattacharjee Anup K.
7. Bidaye A.C.
8. Chakraborty S.P.
9. Chakravartty J.K.
10. Chakravarty Anindya
11. Chattopadhyay J.
12. Chaturvedi Shashank
13. Das Ramakrishna
14. Dey G.K.
15. Dutta B.K.
16. Dwarakanath T.A.
17. Gantayet L.M.
18. Gopalakrishnan Sugilal

19. Gopika Vinod
20. Grover R.B.
21. Gursharan Singh
22. Hubli R.C.
23. Kain Vivekanand
24. Kallol Roy
25. Kapoor Rajeev
26. Kar D.C.
27. Khan K.B.
28. Maheshwari N.K.
29. Mukhopadhyay Sulekha (Ms.)
30. Nayak Arun Kumar
31. Pal Sangita (Ms.)
32. Pal Prabir Kumar
33. Patankar V.H.
34. Prakash Deep
35. Prasad G.J.
36. Ramanathan S.
37. Ravindranath S.V.G.
38. Reddy G.R.
39. Roy . S.B. (Ms.)
40. Roy Debanik
41. Saha Sandip
42. Samal M.K.
43. Saravana Kumar U.
44. Satyamurthy P.
45. Sharma Archana (Mrs.)
46. Singh J.B.
47. Singh R.K.
48. Singh R.N.
49. Singh R.N.
50. Srivastava D.
51. Suri Ashok Kumar
52. Suri Vinod Kumar
53. Taliyan S.S.
54. Tewari P.K.
55. Tewari R.
56. Tiwari A.P.
57. Topkar Anita V. (Ms.)
58. Tripathy P. K.
59. Varde Prabhakar V.
60. Vijayan P.K.
61. Vincent Tessy (Ms.)
62. Vinod Kumar A.

Life Sciences

1. Dr. Apte S.K.
2. Dr. Bandekar J.R.

3.   Dr. Balakrishnan Sreedevi
4.   Dr. Badigannavar Anand
5.   Dr. Ballal Anand
6.   Dr. Chatterjee Suchandra
7.   Dr. Das Birajlakshmi
8.   Dr. Fulzele D.P.
9.   Dr. Ganapathi T.R.
10. Dr. Gautam Satyendra
11. Dr. Gopalakrishnan Roja (Mrs.)
12. Dr. Ghosh Anu
13. Dr. Indira Priyadarshini
14. Dr. Jambhulkar S.J.
15. Dr. Jamdar S. N.
16. Dr. Jawali N.
17. Dr. Joseph Lebana J. (Mrs.)
18. Dr. Kale S.P.
19. Dr. Kulkarni Savita
20. Dr. Melo J.S.
21. Dr. Misra H.S.
22. Dr Mukherjee . P.K.
23. Dr. Mukesh Kumar
24. Dr. Mukopadhyaya Rita
25. Dr. Nancharaiah Y.N.
26. Dr. Pandey B.N.
27. Dr. Patro Birija A.
28. Dr. Rajan M.G.R.
29. Dr. Rajaram Hema
30. Dr. Rao T.S.
31. Dr. Reddy K. S.
32. Dr. Saini Ajay
33. Dr. Samuel Grace
34. Dr. Santosh Kumar S.
35. Dr. Satpathy K.
36. Dr. Shankar Bhavani S.
37. Dr Souframanien . J
38. Dr. Subramanian Mahesh
39. Dr. Suprasanna P.
40. Dr. Sharma A.K.
41. Dr. Variyar Prasad
42. Dr. Venugopalan V.P.
43. Dr. Vinay Kumar

Physical Sciences

1.   Ahmed Zafar
2.   Aswal D.K.
3.   Aswal V.K.
4.   Auluck S.K.H.
5.   Bakshi Ashok Kumar

6.   Bandyopadhyay Tapas
7.   Basu Saibal
8.   Bhanumurthy Karanam
9.   Bhattacharyya Dibyendu
10. Biswas Dhruba J.
11. Biswas Dipak Chandra
12. Chaplot S.L.
13. Chaturvedi Shashank
14. Chauhan A.K.
15. Chougaonkar Mohan Pandharinath
16. Chourasiya G.
17. Das Amitabh
18. Das Asoka Kumar
19. Dasgupta K.
20. Datar V.M.
21. Datta Debabrata
22. Debabrata Biswas
23. Debnath A.K.
24. Degwekar S.B.
25. Deo Mukul Narayan
26. Dutta Dipanwita (Ms.)
27. Gadkari Sanjay C.
28. Gaitonde D.M.
29. Ghorui Srikumar
30. Godbole S.V.
31. Goswami B.K.
32. Gupta Anurag
33. Gupta N.K.
34. Gupta S.C.
35. Gupta Shiv Kumar
36. Jagatap B.N.
37. Jain Sudhir Ranjan
38. John Bency V.
39. Kailas Swaminathan
40. Kannan. Umasankari 9 Ms.)
41. Kaushik T.C.
42. Koul Dileep Kumar
43. Krishnani P.D.
44. Kshirsagar R.J.
45. Kulkarni Mukund S.
46. Kumar Vinay
47. Mahata Kripamay
48. Mala Rao (Ms.)
49. Manohar K.G.
50. Mazumder Subasish
51. Mishra Adya Prasad
52. Mishra D.R.
53. Mitra A.K.
54. Mittal K.C.

55. Mittal Ranjan
56. Mohanty Ajit Kumar
57. Mukesh Kumar
58. Mukhopadhyay Ramaprasad
59. Murali Chitra (Ms.)
60. Nakhate S.G.
61. Nayak B.K.
62. Nilaya J. Padma (Ms.)
63. Palani Selvam T.
64. Pant Lalit Mohan
65. Patil D.S.
66. Pradhan S.
67. Raja Sekhar B.N.
68. Rajarajan A.K.
69. Ramaniah Lavanya M. (Ms.)
70. Rannot R.C.
71. Rao Ms. P.M.
72. Rao Turumella V. Chandrasekhar
73. Ravikumar G.
74. Ray Aditi (Ms.)
75. Roy Bidyut Jyoti
76. Sahoo N.K.
77. Sangeeta (Ms.)
78. Santra Satyaranjan
79. Sapra . B.K. (Ms.)
80. Sarkar P.K.
81. Sathiyamoorthy D.
82. Saxena Alok
83. Sen Debasis
84. Sharma Sunil Dutt
85. Sharma Surinder M.
86. Shrivastava Aradhana
87. Shukla Prashant
88. Singh Pitamber
89. Sinha Sucharita (Ms.)
90. Sinha Amar
91. Suresh Kumar
92. Suryanarayana M.V.
93. Thakur Kiran Balwantrao
94. Tickoo A.K.
95. Umamaheswara Sastry P.
96. Vas Dev
97. Warrier Manoj Kumar
98. Yusuf S.M.

Strategic Studies

1. Grover R.B.
2. Ramakumar K.L.

HRI

Physical Sciences

1. Aditi Sen De (Ms.)
2. Basu Anirban
3. Bhattacharjee J.K.
4. Choubey Sandhya (Ms.)
5. Das Tapas Kumar
6. Datta Aseshkrishna
7. Gandhi Raj
8. Gopakumar Rajesh
9. Jatkar Dileep P.
10. Maharana Anshuman
11. Majumdar Pinaki
12. Mukhopadhyaya B.
13. Naik Satchidanada
14. Pai G. Venketeswara
15. Panda Sudhakar
16. Pareek T.P.
17. Pati Arun Kumar
18. Rai Santosh K.
19. Rao Sumathi (Ms.)
20. Ravindran V.
21. Sen Ashoke
22. Sen Prasenjit
23. Sen Ujjwal
24. Sriramkumar L.

Mathematical Sciences

1. Adhikari Sukumar Das
2. Chakraborty Kalyan
3. Dalawat Chandan Singh
4. Batra Punita
5. Ramakrishnan B.
6. Raghavendra N.
7. Ratnakumar P.K
8. Dey Rukmini
9. Thangadurai R.
10. Ramana Surya
11. Manoj Kumar]
12. Prakash Gyan
13. Shah Hemangi M. (Ms.)

IGCAR

Chemical Sciences

1. Ananthasivan K.
2. Anthonysamy S.
3. Antony M.P.
4. Ganesan Rajesh
5. Ganesan V.
6. Gnanasekaran T.
7. Govindhan Kutty K.V.
8. Jayaraman V.
9. Jena Hrudananda
10. Joseph M.
11. Lakshmi Narasimhan T.S.
12. Mallika C.
13. Mudali U. Kamachi
14. Nagarajan K.
15. Panigrahi Bhabani Shankar
16. Ponraju D.
17. Pujar M.G.
18. Rao P.R. Vasudeo
19. Sai Baba M.
20. Satpathy K.K.
21. Srinivasan T.G.
22. Sundararajan K.
23. Viswanathan R.

Engineering Sciences

1. Albert Shaju K.
2. Anish Kumar
3. Bhaduri Arun K.
4. Chellapandi P.
5. Jayakumar T.
6. Laha Kinkar
7. Mathew M.D.
8. Moitra Aniruddha
9. Mudali U. Kamachi
10. Mukhopadhyay C.K.
11. Muraleedharan P.
12. Murugan S.
13. Parmeswaran P.
14. Ramachandran D.
15. Rao B. Purna Chandra
16. Saroja Saibaba S (Ms.)
17. Sasikala G. (Ms.)
18. Shankar P.
19. Sharma Anil Kumar
20. Sivaprasad P.V.
21. Srinivasan V.S.

22. Swaminathan P.
23. Valsan M.
24. Velusamy K.
25. Venugopal S.

Physical Sciences

1. Amarendra G.
2. Amirthapandian S.
3. Awadhesh Mani
4. Baskaran R
5. Bharathi A.
6. Bhaskaran R.
7. Chandra Shekar N.V.
8. Dasgupta Arup
9. Devan K.
10. Divakar Ramachandran
11. Govindaraj R.
12. Janaki J.
13. John Philip
14. Jose M.T.
15. Kamruddin M.
16. Keshavamurthy R.S.
17. Mangamma G.
18. Mathews Tom
19. Mathi Jaya. S.
20. Nithya Ravindran (Ms.)
21. Panigrahi B.K.
22. Raghavan G.
23. Rajagopalan S.
24. Rajaraman R.
25. Ramaseshan R.
26. Ravindran T.R.
27. Sahu P.Ch.
28. Sairam T.N.
29. Sandip Kumar Dhara
30. Sharat Chandra
31. Sitaram Dash
32. Sivakumar S.
33. Sivasubramanian V.
34. Sridharan V.
35. Srinivas C.V.
36. Subramanian N.
37. Sundar C.S.
38. Sundravel B.
39. Tata B. V. R.
40. Tripura Sundari S.
41. Tyagi A. K.
42. Venkatesan R.
43. Venkatraman B.
44. Vijayalakshmi M.

IMSc

Mathematical Sciences

1. Arvind V.
2. Balasubramanian R.
3. Chakraborty Partha Sarathi
4. Gun Sanoli
5. Iyer Jaya N.
6. Kesavan S.
7. Kodiyalam Vijay
8. Krishna M.
9. Lodaya Kamal
10. Mohari Anilesh
11. Mohari Anilesh
12. Nagaraj D.S.
13. Paranjape Kapil H.
14. Prasad Amritanshu
15. Raghavan K.N.
16. Raman V.
17. Ramanujam R.
18. Sankaran Parameswaran
19. Srinivas Kotyada
20. Subramanian C.R.
21. Sunder V.S.

Physical Sciences

1. Adhikari Ronojoy
2. Anishetty Ramesh
3. Ashok Sujay (Ms.)
4. Date Ghanashyam D.
5. Digal Sanatan
6. Ghosh Sibasish
7. Gopalakrishna Shrihari
8. Govindarajan T.R.
9. Hassan Syed Raghib
10. Indumathi D. (Ms.)
11. Kalyana Rama S.
12. Kaul Romesh
13. Menon G.I.
14. Mishra Ashok Kumar
15. Menon gautam I.
16. Murthy M.V.N.
17. Mukhopadhyay Partha
18. Nemani Venkata S.
19. Rajesh Ravidran
20. Ray Purusattam

21. Sathiapalan Balachandran
22. Shankar R.
23. Sharatchandra H.S.
24. Siddharthan Rahul
25. Simon R.
26. Sinha Nita (Ms.)
27. Sinha Rahul
28. Sinha Sitabhra
29. Vemparala Satyavani (Ms.)

Engineering Sciences

1. Mahajan M.B. (Ms.)
2. Raman V.
3. Subramanian C.R.

Life Sciences

1. Vemparala Satyavani
2. Sinha Sitabhra
3. Siddharthan Rahul

IPR

Engineering Sciences

1. Pathak Surya Kumar
2. Shyam Anurag
3. Mukherjee Subroto

Physical Sciences

1. Amita Das (Ms.)
2. Awasthi Lalit Mohan
3. Bandopadhyay Mainak
4. Bandyopadhyay Pintu
5. Bora Dhiraj
6. Chandra Debasis
7. Chattopadhyay Asim Kumar
8. Chattopadhyay P.K.
9. Deshpande Shishir P.
10. Ganesh Rajaraman
11. Ghosh Joydeep
12. Jha Ratneshwar
13. Joshi Hem Chandra
14. Karkari Shantanu Kumar

15. Kaw P.K.
16. Khirwadkar Samir S.
17. Kulkarni Sanjay V.
18. Kulkarni Sanjay V.
19. Kumar Ajai
20. Kumar Vinay
21. Kundu Mrityunjay
22. Mohanty Smruti R.
23. Mukherjee Subroto
24. Pradhan Subrata
25. Pradhan Subrata
26. Raju Daniel
27. Ramasubramanian N.
28. Raole P.M.
29. Reddy D.Chenna
30. Sen Abhijit
31. Sengupta Sudip
32. Sharma Pramod Kumar
33. Shyam Anurag
34. Singh Raghevendra
35. Srinivasa Rao C.V.
36. Srinivasan R.
37. Tanna Vipulkumar L.

IoP

Physical Sciences

1. Agarwalla Sanjib
2. Agrawal Pankaj
3. Bhattacharjee Somendra Mohan
4. Dev Bhupendra Nath
5. Jayannavar A.M.
6. Mukherji Sudipta
7. Ota Shehadri B.
8. Patra Suresh Kumar
9. Satyam Parlapalli Venkata
10. Sekhar Biju R.
11. Som Tapobrata
12. Srivastava Ajit Mohan
13. Topal Dinesh K.
14. Tripathy Goutam
15. Varma Shikha
16. Virmani Amitabh

RRCAT

Physical Sciences

1. Banerjee Arup
2. Bartwal K.C.
3. Bindra Kushvinder Singh
4. Chakera J.A.
5. Chakrabarti Aparna
6. Chattopadhyay Maulindu Kumar
7. Dixit S.K.
8. Dixit V.K.
9. Ganesamoorthy S.
10. Ganguli Tapas
11. Ghosh Haranath
12. Gupta P.K.
13. Gupta Parshotam Dass
14. Gupta Surya Mohan Ingale Alka (Ms.)
15. Joshi Mukesh
16. Karnal A.S.
17. Kukreja L.M.
18. Lodha G.S.
19. Majumder S.K.
20. Mishra Satya Ram
21. Modi Mohammed Hussein
22. Moorti Anand
23. Mukherjee C.
24. Mukhopadhyay P.K.
25. Naik Prasad Anant
26. Oak S.M.
27. Om Prakash
28. Rai V.N.
29. Rama Chari
30. Rawat H.S.
31. Roy Sindhunil Barman
32. Senecha V.K.
33. Shailendra Kumar
34. Sharma Avnish K.
35. Sharma Tarun Kumar
36. Singh Chandra Pal
37. Singh Manoranjan P.
38. Sinha A.K.
39. Srivastava Arvind Kumar
40. Tiwari Manoj Kumar
41. Tiwari Vidya Sagar
42. Vinit Kumar

Engineering Sciences

1. Chatterjee Sanjib
2. Paul C.P.

Life Sciences

1. Dube Alok
2. Mrinalini Sharma. S. (Ms.)

SINP

Chemical Sciences

1. Basu Samita (Ms.)
2. Bhattacharyya Dhananjay
3. Chakrabarti Abhijit
4. Ganguly B. (Ms.)
5. Hazra Montu K.
6. Lahiri Susanta
7. Mishra Padmaja P. (Ms.)
8. Sarkar Munna

Engineering Sciences

1. Mukhopadhyay S.

Life Sciences

1. Banerjee Rahul
2. Banerjee Subrata
3. Bhattacharyya Dhanjay
4. Bhattacharyya Nitai Pada
5. Biswas Sampa
6. Chakrabarti Chandana (Ms.)
7. Chakrabarti Oishee (Ms.)
8. Chakrabarti Abhijit
9. Chakrabarti Abhijit
10. Das Chandrima
11. Dasgupta Dipak
12. Mukhopadhyay Debashis
13. Saha Partha
14. Sen Udayaditya

Physical Sciences

1. Agrawal Bijay Kumar
2. Bandyopadhyay Bilwadal
3. Banerjee Polash
4. Banerjee S.
5. Banerjee Sunanda
6. Basu Chinmay
7. Basu Padmanava
8. Bhattacharjee P.
9. Bhattacharya Satyaki
10. Bhattacharyya G.

11. Bhattacharyya S.R.
12. Bhunia Satyaban
13. Chakrabarti Bikas Kanta
14. Chakrabarti Nikhil
15. Chakraborty Nikhil
16. Chakraborty Purushottam
17. Charan Dey Chandi
18. Das Atindra Nath
19. Das Debasish
20. Das Indranil
21. Das Mala (Mrs.)
22. De Asit K.
23. De Sankar
24. Dutta Suchandra
25. Ganguly Bichitra
26. Ghosh Amit
27. Ghosh Debabrata
28. Goswami Ashimananda
29. Gupta Kumar S.
30. Harindranath A.
31. Iyengar A.N. Sekar
32. Janaki M.S. (Mrs.)
33. Kundu Anjan
34. Majumdar Debasish
35. Majumdar Parthasarathi
36. Majumdar Pratik
37. Mallick Bireswar Basu
38. Mandal Prabhat K.
39. Mazumdar Abhee Kanti Dutt
40. Mazumdar Chandan
41. Menon Krishnakumar S.R.
42. Mitra Parathasarathi
43. Mukherjee Anjali (Ms.)
44. Mukherjee Chandidas =
45. Mustafa Munshi Golam
46. Pramanik Ushasi Datta
47. Ray Kajal Ghosh (Mrs.)
48. Roy Pradip Kumar
49. Roy Sibaji
50. Roy Subinit
51. Saha Satyajit
52. Samanta Chhanda
53. Sanyal Milan Kumar
54. Sarkar Maitreyee Saha
55. Sarkar Sandip
56. Sarkar Subir
57. Satpati Biswarup
58. Sengupta Dr. K.
59. Singh H.
60. Sinha Tinku (Ms.)

TMC

Chemical Sciences

1. Pakhale S.S.

Life Sciences

1. Joshi Narendra N.
2. Kelkar Rohini S. (Ms.)
3. Narkar. A.A. (Ms.)
4. Shrivastava S.K.
5. Waghmare Sanjeev K.
6. Jambhekar N.A.
7. Arya Supreeta (Ms.(
8. Baksh Sumitra G. (i Ms.)
9. Bhattacharyya Dibyendu
10. Bose Kakoli
11. Chandan Kumar
12. Chiplunkar S.V. (Ms.)
13. Dalal S.N.
14. De Abhijit
15. Deodhar Kedar K.
16. Desai S.B. (Ms.)
17. Desai S.M. (Ms.)
18. Dinshaw K.A.
19. Dixit Rajesh
20. Dutt Amit
21. Dutt Shilpee (Ms.)
22. Engineer Reena (Ms.)
23. Ganesh B.
24. Gota Vikram Gude Rajiv P.
25. Gupta Sanjay
26. Gupta Tejpal
27. Joseph Lebana J. (Ms.)
28. Kadam P.S. Amare (Ms.)
29. Kalraiya Rajiv D.
30. Krishna C.M.
31. Kulkarni P.G.
32. Laskar Sarbani Ghosh (Ms.)
33. Mahantshetty Umesh M.
34. Mahimkar Manoj B.
35. Mallath M.K.
36. Maru Girish B
37. Mukhopadhyaya Rabindranath
38. Mulherkar Rita (Ms.)
39. Myatra Sheila N. (Ms.)
40. Naik Nishigandha R. (Ms.)
41. Pakhale Shrirang Shankar
42. Rai Rekha (Ms.)
43. Ramadwar Mukta (Ms.)
44. Ramani S.K.
45. Ray Pritha
46. Sarin Rajiv
47. Shastri S.S.
48. Shirsat Neelam Vishwanath
49. Teni Tanuja R. (Ms.)
50. Thakur M.H.
51. Vaidya Milind M.
52. Varma Ashok K.
53. Venkatraman Prasanna
54. Zingde S.M.

Health Sciences

1. Agarwal Jai Prakash
2. Deshpande D.D.

VECC

Chemical Sciences

1. Sen Pintu

Engineering Sciences

1. Mukherjee Paramita
2. Pal Sandip
3. Sarkar Debranjan

Physical Sciences

1. Ahammed Zubayer
2. Bandyopadhyay S.K.
3. Banerjee Gayathri N.(Ms.)
4. Banerjee S.R.
5. Barat P.
6. Basu D.N.
7. Bhandari Rakesh Kumar
8. Bhattacharya Mishreyee (Ms.)
9. Bhattacharya S.
10. Bhattacharyya Sarmishta
11. Bhattcharya Chandana (Ms)
12. Bhowmick Debasis
13. Chakrabarti Alok
14. Chattopadhyay S.
15. Chaudhuri A.K.
16. Chaudhuri Gargi (Ms.)
17. Das Nishit Kumar
18. Das Parnika (Ms.)
19. De U.

20. Ghosh Premomoy
21. Ghosh Tilak Kumar
22. Jan-e-Alam
23. Karmakar Prasanta
24. Mohanty B.
25. Mukherjee Gopal
26. Mukhopadhyay Tapan
27. Naik Vaishali (Ms.)
28. Pal Santanu
29. Pandit Vijay Shanker
30. Rashid M.H.
31. Ray A.
32. Sanyal Dirtha
33. Sarkar S.
34. Sarma P.R.
35. Srivastava D.K.
36. Tapan Kumar Nayak
37. Viyogi Y.P.

NISER- IoP

Chemical Sciences

1. Arunachalam S.
2. Barman Sudip
3. Behera Jogendra N.
4. Bhargava B.L.
5. Chandrashekar T.K.
6. Das Ritwick
7. Ghosh Arindam
8. Ghosh Subhadip
9. Gunanathan C.
10. Kar Sanjib
11. Krishnan V.
12. Lourderaj Upakarasamy
13. Nembenna S.
14. Peruncheralathan S.
15. Prasenjit Mal
16. Purohit Chandra S.
17. Sarkar Moloy
18. Sharma Nagendra K.
19. Srinivasan A.

Physical Sciences

1. Anil Kumar A.V.
2. Basak Subhasish
3. Bedanta Subhankar

4. Benjamin Colin
5. Bhattacharjee Joydeep
6. Chandra V. Ravi
7. Gowdigere Chetan N.
8. Mal Prolay Kumar
9. Mohapatra Ashok
10. Moloy Sarkar
11. Moulik Tania
12. Nagendra K. Sharma
13. Sahoo Pratap Kumar
14. Samal Prasanjit
15. Senapati K.
16. Srinivasan A.
17. Srivastava Yogesh K.
18. Sumedha (Ms.)
19. Swain Sanjay Kumar

Mathematical Sciences

1. Dalai Deepak Kumar
2. Jana Nabin Kumar
3. Karn Anil Kumar
4. Muruganandam V.
5. Parui Sanjay
6. Patra Kamal L.
7. Sahoo Binod Kumar

Life Sciences

1. Acharya Rudresh
2. Aich Palok
3. Alone Debasmita P.
4. Alone Pankaj V.
5. Bagchi Sumanta
6. Bhattacharyya Asima (Ms.)
7. Chattopadhyay Subhasis
8. Chowdary T.K.
9. Dixit Ms. Manjusha
10. Goswami Chandan
11. Konkimalla V.S.B.
12. Mohapatra Harapriya
13. Panigrahi Kishore
14. Rahaman Abdur
15. Shrivastav Anurag
16. Singru Praful S.

Annex 4

Admission and Results Status

(April 1, 2012 – March 31, 2013)

HOMI BHABHA NATIONAL INSTITUTE
Admissions : 2012

S.No.	Programme	BARC	IGCAR	RRCAT	VECC	SINP	IPR	IOP#	HRI	TMC	IMSc	TOTAL
1	PGD*	34	18									52
2	PGDRM	4										4
3	PGDMRIT	9										9
4	DipRP	27										27
5	I. M.Sc.$											0
6	M. Sc. Engg.)	6	4									10
7	M. Tech.#	222	49	23	1							295
8	M. Phil.#											0
9	Ph. D. Engg.)	28	22	1								51
10	Ph. D. (Phys.)	19	19	19	10		14	18	10		7	116
11	Ph. D.Chem.)	22	11	1				9				43
12	Ph. D. (Life)	9						5		13		27
13	Ph. D. Math.)								4		6	10
14	Ph. D. (Hlth.)									5		5
15	Ph. D. (Stra.)											0
16	I. PhD (Phys.)								6		12	18
17	I. PhD Math.)										4	4
18	M. Ch.									17		17
19	M. D.									39		39
20	D. M.									15		15
21	C. Fellowship									18		18
22	Nursing									8		8
Total		380	123	44	11	0	14	32	20	115	29	768

Actual Admission No.: Total-(MTech+MPhil) No.= 473
includes NISER enrolments
PGD: Post Graduate Diploma in Nuclear Science and Engineering
DRM: Diploma in Radiation Medicine, DMRIT: Diploma in Medical Radio Isotope Techniques
Dip. R. P.: Diploma in Radiological Physics
M. Tech: Master of Technology, M. Phil: Master of Philosophy
I. M.Sc.: Integrated M. Sc. at NISER under IoP
M. Sc. (Engg.): Master of Science (Engineering)
Ph. D.: Engineering, Physics, Chemistry, Life, Mathematics, Health and Strategic Studies, IPhD: Integrated Ph. D.
M. Ch.: Surgical Oncology, MD: Pathology, Radiotherapy, Radiodiagnosis, Anaesthesia
DM: Medical Oncology
C. Fellowship: Certified Fellowship programme of 2 Years under Health Sciences
Nursing : M.Sc. (Nursing) programme of 2 years under Health Sciences
Refers to Students who have upgraded enrolment from PGD to M. Tech./ M. Phil.
    subsequent to successfully completing course work for PGD

Note: All OCES Engg. Students enrolled directly under Mtech from 2012, but the total here OCES-2012 Mtech enrolment
        NO.= 200 also reflects OCES-2011 PGD students

Results declared during April 1, 2012 – March 31, 2013

COM-9

Sr.No.	Degree/Diploma	No.
1.	PGD	45
2.	M. Tech.	154
3.	M. Sc.(As part of Int. Ph. D.)	12
4.	M. Sc. (Engg.)	7
5.	Ph. D.	38
6.	M.D.	1
7.	DRM	2
8.	DMRIT	0
9.	Dip. R. P.	24
Total		**283**

COM-10

Sr.No.	Degree/Diploma	No.
1.	M. Tech.	15
2.	M. Sc. (Integrated)NISER-1st Batch	35
3.	M. Sc. (Engg.)	1
4.	M. Phil.	1
5.	Ph. D.	14
6.	DRM	4
7.	DMRIT	6
Total		**76**

COM-11

Sr.No.	Degree/Diploma	No.
1.	M. Tech.	99
2.	M. Sc. (Engg.)	3
3.	M. Sc.(As part of Int. Ph. D.)	1
4.	Ph. D.	65
5.	Dip. R. P.	30
6.	MD	17
7.	DM	5
8.	MCh	2
9.	Fellowship	18
Total		**240**

Note : As and when a student completes all academic requirements of a programme, his/her result is notified. Results are declared after approval by CoM.

Annex 5

Abstracts of Ph.D. Theses

(April 1, 2011 to March 31, 2012)

Name	:	**Amit Das**
Enrolment No.	:	CHEM0120804014
Constituent Institute	:	Institute of Physics, Bhubaneswar
Title		X-Ray Crystallographic Studies on HIV-1 Protease

Abstract

The unique contribution of the candidate is structural mapping of the peptide bond cleavage reaction catalyzed by HIV-1 protease (HIV-1 PR). The candidate has obtained the first crystal structures of complexes between an active HIV-1 PR enzyme and natural type-1 and type-2 substrates. In the complexes with a type-2 substrate, the substrate is captured in the active site at three different stages of the cleavage reaction: when bound as a regular peptide, after *in-situ* modification into a tetrahedral reaction intermediate, and when cleaved into product peptides, which are still bound in the active site of the enzyme. He has discovered an inter-enzyme-substrate short ionic hydrogen bond (SIHB) in the tetrahedral intermediate complex, and an intra- enzyme low barrier hydrogen bond (LBHB) just after the substrate is cleaved into product peptides. In the complex with type-1 substrate, the substrate is cleaved and the C-terminal peptide bond about the proline residue displays *cis* conformation. These are very novel and atomic level descriptions of substrate recognition and processing by HIV-1 protease enzyme. Based on these structural inputs he has given a detailed mechanism of the peptide bond hydrolysis by HIV-1 PR. Through very high resolution structures, the candidate has found that in unliganded HIV-1 PR, the inter-aspartate hydrogen bond is not a LBHB, in contradiction to the latest mechanistic proposal. Further, the candidate has found novel arrangement of water molecules at the catalytic centre, only when the pH is non-optimal for enzyme activity. The rate reduction at non-optimal pH's is suggested to be partly due to this water structure. The candidate has also determined the structures of the complexes of FDA approved drug, ritonavir with native as well as HIV-1 PR mutants that are resistant to ritonavir. These structures reveal that, in V82F mutant, loss of hydrophobic interactions contributes significantly toward development of resistance and the M36I mutant has a compensatory role in restoring viral fitness. Two datasets were collected remotely from HBNI using the FIP beamline at ESRF.

Publications

1. Amit Das, S.Bihani, V.Prashar, J.-L.Ferrer and M.V.Hosur; "Crystal structures of complexes of wild-type and V82F mutant HIV-1 Protease with ritonavir - insights into drug resistance." Manuscript submitted for publication.

2. 2. Amit Das, J.-L.Ferrer and M.V.Hosur; "X-ray snapshots of HIV-1 protease catalysis and substrate recognition"; Acta Crystallographica (2011), A67, C425.

3. Amit Das, S.Mahale, V.Prashar, S.Bihani, J.-L.Ferrer and M.V.Hosur; "X-ray snapshot of HIV-1 protease in action: observation of tetrahedral intermediate and its SIHB with catalytic aspartate"; Journal of American Chemical Society (2010), 132, 6366-6373. This paper has been selected to be published in JACS Select, 2011.

4. Amit Das, D.R.Rao and M.V.Hosur; "X-ray Structure of HIV-1 Protease Tethered Dimer Complexed to Ritonavir"; Protein and Peptide Letters (2007), 14, 565-568.

5.   Amit Das, V.Prashar, S.Mahale, J.-L.Ferrer, L.Serre and M.V.Hosur; "X-ray structure of insitu HIV-1 protease-product complex: observation of a LBHB between catalytic aspartates"; Proceedings of National Academy of Sciences, USA (2006), 103 (49), 18464-18469.

6.   S.Bihani, Amit Das, V.Prashar, J.-L.Ferrer and M.V.Hosur; "X-ray structure of in-situ HIV-1 protease-product complex"; Proteins: Structure, Function and Bioinformatics (2008), 74(3), 594-602.

7.   V.Prashar, Amit Das, S.C.Bihani, J.-L.Ferrer and M.V.Hosur "Catalytic water co-existing with product peptide in the active site of HIV-1 Protease: Insights into the reaction mechanism"; PLoS One (2009), 4(11), e7860, 1-8.

List of symposia presentations, conferences, etc.:

1.   M.V. Hosur, S.Bihani, V.Prashar and Amit Das; "X-ray structures of drug resistant HIV-1 protease and drug complexes"; Indo-US symposium/Workshop, Modern Trends in Macromolecular Structures, IL-29, Indian Institute of Technology, Mumbai, India (2011).

2.   2. Amit Das, M.V.Hosur, V.Prashar and S.Bihani; European Molecular Biology Symposium, Recent advances in Macromolecular Crystallography, National Chemical Laboratory, Pune, India (2008).

3.   3. M.V.Hosur, Amit Das, V.Prashar and S.Bihani; "Structural investigations of HIV-1 Protease complex with substrates and inhibitors"; 37th National Symposium on Crystallography, Jadavpur University, Kolkata, India (2008).

4.   M.V.Hosur, Amit Das and V.Prashar; "Structure of a tethered dimer of HIV-1 protease complexed to a decapeptide corresponding to a RT-RH junction"; Joint Conference of the Asian Crystallographic Association and the Crystallographic Society of Japan, Epochal Tsukuba, Japan (2006).

5.   M.V.Hosur, B.Pillai, M.Kumar, V.Prashar, Amit Das, S.C.Bihani and S. Mahale; "X-ray structures of HIV-1 protease substrate complexes"; International Symposium on Emerging Trends in Genomic and Proteomic Sciences, National Institute of Reproductive Research and Health (ICMR), Mumbai, India (2006).

6.   Amit Das, V.Prashar and M.V.Hosur; "Structure of a tethered dimer of HIV-1 protease complexed to a decapeptide corresponding RT-RH junction"; National Seminar on Crystallography, National Physical Laboratory, New Delhi, India (2006).

7.   M.V. Hosur, B.Pillai, M.Kumar, V.Prashar, Amit Das and S.Mahale; "Structures of HIV-1 protease complexed to peptide substrates"; Indian Biophysical Society symposium, Kolkata, India (2006).

Name	:	**Binata Panda**
Enrolment No.	:	PHYS0720060421
Constituent Institute	:	Institute of Physics, Bhubaneswar
Title		Phenomenology with Magnetized D-Branes

Abstract

Superstring theory is currently considered to be one of the most promising candidates for unifying the different particles and their interactions in nature. The search for realistic string vacua is one of the most ambitious tasks in Superstring theory. A phenomenologically viable string compactification should contain three chiral fermion generations, the Standard Model gauge group or some extension of it e.g. GUTS models and broken space-time supersymmetry. In addition to this basic structure, it should reproduce the exact gauge and Yukawa couplings. Moreover, it should satisfy a set of conditions in order to produce a consistent anomaly free theory. Further, all the moduli, unobserved massless scalar fields, are needed to be stabilized. In the present thesis, we discuss a simple framework of toroidal compactification of type I string theory with magnetized (D-branes with worldvolume fluxes along compactified tori), that offers an interesting self-consistent set up for string phenomenology. We begin with a discussion of comactification of type 1 string on a torus with additional background gauge flux on the D9-branes and review the necessary constructing semi-realistic models in such a framework. We then carry the computations of Yukawa coupling in such magnetized brane constructions. The fermion (scalar) wavefunctions on toroidally compactified spaces are presented for general fluxes. By evaluation the overlap integral of the wave functions, the close form expressions for Yukawa coupling among chral multiplets are obtained. This essentially leads us to construct certain mathematical identities for general Riemann theta functions. Finally, we present a minimal example of a sypersymmetric grand unified model in a toroidal compactification of type 1 stirng theory with magnetized D9-branes. The gauge symmetry is just SU (5) and the gauge non-single chiral spectrum contains only three families of quarks and leptons transforming in the 10+ $\bar{5}$ representations. All geometric moduli are stabilized in terms of the background internal magnetic fluxes. Further, using the results for Yukawa coupling, we discuss the mass generation for several non‾chiral fermion muliplets in a supersymmetric ground state.

Publications

1. "Supersymmetric SU(5) GUT with stabilized modul", Ignations Antoniadis, Alok Kumar, Binata Panda, Nucleal Physics B 795 (2008) 69 [arXiv:0709.2799[hep‾th,hep-ph]].

2. "Fermion Wavefunctions in Magnetized branes: Theta identities and Yukawa Coupling", Ignations Antoniadis, Alok Kumar, Binata Panda, Nuclear Physics B 823 (2009) 116 [arXiv:0904.0910[hep-th,hep-ph]].

3. "Brane Embeddings in AdS$ _4 $ × CP$ 3 $'', B. Chandrasekhar, Binata Panda, Int. J. Mod. Phys. A 26 (2011) 2377 [arXiv:0909.3061[hep-th]].

4. "Black hole phase transitions via Bragg-Williams", Souvik Banerjee, Sayan K. Chakrabarti, Sudipta Mukherji, Binata Panda, Int. J. Mod. Phys. A26 (2011) 3469 [arXiv:1012.3256 [hep-th].

Name	:	**Ashish Kumar Srivastava**
Enrolment No.	:	LIFE01200604007
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Identification of Thiol Induced Transcripts, Their Functional Characterization and Role in Crop Improvement

Abstract

Salinity as an important abiotic environmental stress has become a major limitation for plant growth and crop production worldwide. Earlier research in our laboratory has identified thiourea (TU) for enhancing the plant's stress tolerance and crop productivity under field conditions. The present work was undertaken to unravel the molecular mechanisms or TU-mediated action. The differential display was performed in Indian mustard (Brassica juncea L.) seeds subjected to distilled water (control), NaCl, NaCl+TU and TU treatments and the data suggested the significane of mitochondrial ATPase in TU-mediated maintenance of seed germination ability under salt stress. The microarray analysis revealed the differential expression profile of 33 genes in NaCl with/without TU treatment which were established as markers of tress tolerance. The real-time RT-PCR and related biochemical studies were conducted to validate differential display and microarray data. The addition of $LaCl_3$ (a specific calcium channel blocker) restricted the responses of TU at molecular and biochemical level suggesting the involvement of cytosolic calcium burst. The TU alone treatment was comparable to that of control. The ameliorative effect of TU was also demonstrated at the seedling stage. The TU treatment differentially modulated the expression of 13 aquaporin isoforms in a time dependent manner. The ^{31}P-NMR studies demonstrated the positive role of TU in maintaining the cytosolic/vacuolar pH gradient. The NaCl+TU treatment reduced the ROS load in the shoot part which helps in maintaining the reduced redox state under NaCl stress. This curtailed the requirement to stimulate different antioxidants. Owing to this, plants were able to channel their energy towards Na^+-ion exclusion/avoidance. Thus, the present thesis deals with both basic and applied aspects, by not only addressing different components of salt tolerance but also ensures the use of TU as a "Bioregulatory technology" for crop improvement.

Publications

[A] Papers published in peer-reviewed International Journal

1. Srivastava AK, Srivastava S, Suprasanna P, D'Souza SF (2011) Thiourea orchestrates regulation of redox state and antioxidant responses to reduce the NaCl-induced oxidative damage in Indian mustard (*Brassica juncea* L.). Plant Physiology and Biochemistry 49, 676-686.

2. Srivastava AK, Ramaswamy NK, Suprasanna P, D'Souza SF (2010) Genome-wide analysis of thiourea modulated salinity-stress responsive transcripts in seeds of *Brassica juncea* L.: Identification of the signaling and effector components of stress tolerance. Annals of Botany (London) 106, 663-674.

3. Srivastava AK, Suprasanna P, Srivastava S, D'Souza SF (2010) Thiourea mediated regulation in the expression profile of aquaporins and its impact on water homeostasis under salinity stress in *Brassica juncea* roots. Plant Science 178, 517-522.

4. Srivastava AK, Ramaswamy NK, Mukopadhyaya R, Chiramal Jincy MG, D'Souza SF(2009) Thiourea modulates the expression and activity profile of mtATPase under salinity stress in *Brassica juncea* L. Annals of Botany (London) 103, 403-410.

[B] Reports

1. Srivastava AK, Ramaswamy NK, D'Souza SF (2008) Bioregulatory role of "thiourea" in multistress tolerance of the Indian mustard (*Brassica juncea*). Founder's Day special issue of BARC News Letter Issue No. 297.

[C] Abstracts presented in national and international conferences

1. Srivastava AK, Suprasanna P, Ramaswamy NK, D'Souza SF (2010) Molecular and biochemical investigation of thiourea mediated responses reveals various signaling and 147 | Page effector components of salinity stress tolerance. [Poster presented in Cold Spring Harbour Symposium on "From Plant Biology to Crop Biotechnology" held at Suzhou, China during October 25-29, 2010].

2. Srivastava AK, Suprasanna P, Srivastava S, D'Souza SF (2009) Thiourea mediates regulation of water homeostasis and expression profile of different aquaporin isoforms in roots of *Brassica juncea* under salt and multistress. Accepted for Poster presentation in 9th International Plant Molecular Biology Congress held at St. Louis, USA during October 25- 30, 2009.

3. Srivastava AK, Ramaswamy NK, D'Souza SF (2007) Rapid transcriptome changes induced by thiourea reveal the role of calcium and calmodulin related proteins in multistress tolerance of *Brassica juncea*. Poster Presented in International symposium on "Calcium based signaling systems in plants" held at Dublin, Ireland during 5th-7th December, 2007 {Received New Phytologist Trust award}.

4. Srivastava AK, Ramaswamy NK, D'Souza SF (2007) Regulatory role of mtATPase subunits of *Brrasica juncea* identified through differential display and quantitative Real-time PCR. Oral Presentation in International symposium on "Light and Life" held at University of Hyderabad 29th -31st August, 2007.

[D] Gene Bank Submissions

1. EU143655; EU143656; EE191543; EE111314; EE111313; FJ654732; GQ243695; GQ243696; GQ243697; GQ243698; GQ243700; GQ243701; GQ243702; GQ243703.

Name : **Prasuna Koshy**
Enrolment No. : CHEM01200604002
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Structural Evaluation in Surfactant Assemblies and Their Application in Nanomaterials Synthesis for Biomedical Application

Abstract

Chapter 1: It contains brief introduction about surfactants, their classifications and various applications. Also a detailed discussion on the factors affecting the structure of surfactant assemblies has been done.

Chapter 2: It deals with the experimental methods and characterization techniques employed in the present study. A brief discussion regarding various instrumental methods, such as dynamic light scattering (DLS), small angle neutron scattering (SANS), Rheology, Cryo transmission electron microscopy (Cryo-TEM), UV-visible spectroscopy, amperometry has been done.

Chapter 3: This chapter describes the effect of chain length on the growth behavior of cetyltrimenthylammonium bromide/ Tetradecyltrimenthylammonium bromide-sodium laurate mixed miscellar systems. Also, from the electrolyte effect on the equilibrium area per monomer, the contributions from steric and electrostatic effects has been separted.

Chapter 4: In this chapter, rheological behavior of linear and branched wormlike micelles formed in mixtures of cetyltrimethylammonium bromide (CTAB) and sodium oleate (NaOL) has been discussed. Scaling of the rheological parameters of CTAB-NaOL catanionic mixtures, as a function of concentration, Employing dynamic rheological measurements has been determined and compared with the predictions of existing scaling laws.

Chapter 5: This chapter describes the dilution induced changes in the microstructure of micelles formed by a cationic surfactant-anionic hydrotrope mixture in the surfactant-rich region. The surfactant used is cetyltrimethylammonium bromide (CTAB) and the hydrotropic salt is sodium 3-hydroxynaphthalene 2-carboxylate (SHNC).

Chapter 6: This chapter describes the preparation of nanoparticles of polyaniline using mixed micelles of sodium dodecyl sulphate (SDS) and anilinium hydrochloride (AHC) as the template. Also the interaction of proteins like progesterone antibody and antigens with polyaniline has been discussed using Interdigitated array (IDA) silver microelectrodes and pulsed amperometric measurements.

Chapter 7: The presentation was concluded by summary of the work.

The presentation was followed by an extensive question answer session, in which wide range of questions were asked by the external examiner, doctoral committee members and other scientists who were present in the audience. She answered all the questions satisfactorily.

Publications

1. Viscoelastic Fluids Originated from Enhanced Solubility of Sodium Laurate in Cetyl Trimethyl Ammonium Bromide Micelles through Cooperative Self-Assembly Prasuna Koshy, Gunjan Verma, V. K. Aswal, Meera Venkatesh and P. A. Hassan *J. Phys. Chem. B*, 2010, 114, 10462-10470.

2. Swelling and Elongation of Tetradecyltrimethylammonium Bromide Micelles Induced by Anionic Sodium Laurate Prasuna Koshy, V. K. Aswal, Meera Venkatesh and P. A. Hassan *Soft Matter*, 2011, 7, 4778-4786.

3. Unusual Scaling in the Rheology of Branched Wormlike Micelles Formed by Cetyltrimethylammonium Bromide and Sodium Oleate Prasuna Koshy, V. K. Aswal, Meera Venkatesh and P. A. Hassan *J. Phys. Chem. B*, 2011, 115, 10817-10825.

4. Dilution Induced Structural Transition in DTAB/SHNC Mixed Surfactant System Prasuna Koshy, V. K. Aswal, Janaky Narayanan, Jayesh Bellare, Meera Venkatesh and P. A. Hassan (Manuscript under preparation)

5. Vesicle Formation in Mixtures of CTAB and Sodium Oleate: Phase behavior and scattering studies. Prasuna Koshy, V. K. Aswal, Meera Venkatesh and P. A. Hassan (Manuscript under preparation)

Name	:	**Bhaskar Sanyal**
Enrolment No.	:	LIFE01200804007
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Studies on Detection and Dosimetry of Irradiated Food by Thermoluminescence(TL) and Electron Paramagnetic Resonance (EPR) Spectroscopy

Abstract

Food irradiation is the treatment of food by ionizing radiation. The need for reliable and routine tests to determine whether or not food has been irradiated has arisen as a result of the progress made in commercialization of the food irradiation technology, increased international trade in irradiated foods, and consumer demand for clear labeling of the treated food. On the other hand, the effectiveness of processing of food by ionizing radiation depends on proper delivery of absorbed dose and its reliable measurement. External influences such as the temperatures of dose measurement, accuracy in a rather narrow dose range are the other problems that confront dosimetry. An attempt has been made to study the identification methodology of irradiated foods with commercially relevant doses based on physical methods namely, Thermoluminescence (TL) measurements and Electron Paramagnetic Resonance (EPR) spectroscopy. In case of measurements of absorbed dose, investigations were carried out to understand the mechanism of modified $CaSO_4$ based thermoluminescence phosphors by TL-EPR correlation studies and to find out the efficacy of the phosphor as a food irradiation dosimeter.

In case of identification of irradiated food, foods were chosen from all the groups of different purposes of irradiation namely sprout inhibition, insect disinfestations, microbial decontamination etc. In many cases both the techniques were employed to give a complete verdict about irradiation. EPR spectroscopy determined various paramagnetic centres namely carbohydrate radical, cellulosic radical and axially symmetric CO_2^- radical ion as the markers of radiation treatment. EPR spectral behavior, relaxation characteristics, and thermal behavior of the radical emerged as useful tools to detect irradiation even after prolonged storage. TL measurements of the isolated minerals from the foods were successfully employed to detect a wide spectrum of irradiated food.

In case of dosimetry of the irradiated foods at sub-ambient temperatures, post-preparation thermal treatments of $CaSO_4$: Dy phosphor revealed structural change in TL glow curve exhibiting increased sensitivity of the low temperature peak that could be usefully exploited for low temperature dosimetry. On the other hand, reduction in TL sensitivity and glow curve structure with increase in Bi concentration in $CaSO_4$: (Dy, Bi) was attributed to the quenching action of Bi^{3+} ions on the TL. The study also suggested that $CaSO_4$: (Dy, Bi) (Bi concentration 0.5 mol %) could be used as a suitable dosimeter in food irradiation dosimetry.

Publications

1. Bhaskar Sanyal, S P Chawla, Arun Sharma. (2011). An improved approach to identify irradiated dog feed by electron paramagnetic resonance study and thermoluminescence measurements. Radiation Physics and Chemistry. Vol. 80: pp of 650 – 657.

2.   Bhaskar Sanyal, V. Natarajan, S. P. Chawla, Arun Sharma. (2010). TL and EPR studies of CaSO4: Dy phosphor to investigate its efficacy in measurement of food irradiation dose at sub-ambient temperatures. Radiation Measurements. Vol. 45: pp of 899 – 905.

3.   Bhaskar Sanyal, Arun Sharma. (2009). A new electron paramagnetic resonance method to identify irradiated soybean. Journal of Food Science. Vol. 74 Nr 8: pp of 57-64.

4.   Bhaskar Sanyal, S. P. Chawla, Arun Sharma. (2009). An improved method to identify irradiated rice by EPR spectroscopy and Thermoluminescence measurements. Food Chemistry. Vol. 116 (2): pp of 526 – 534.

5.   Bhaskar Sanyal, M. G. Sajilata., S. Chatterjee.; R. S. Singhal, P. S. Variyar, M. Y. Kamat, Arun Sharma. (2008). Identification of irradiated cashew nut by electron paramagnetic resonance spectroscopy. Journal of Agriculture and Food Chemistry. Vol. 56: pp of 8987-8991.

6.   A.K. Bakshi, Bhaskar Sanyal, V J Joshi, M K Bhide, V Natarajan and Arun Sharma. (2011). EPR-TL correlation studies on Bi co-doped CaSO4: Dy phosphor. Applied Radiation and Isotope. 69, pp of 254 – 260.

7.   Bhaskar Sanyal, S. P. Chawla, Arun Sharma. (2010). Thermoluminescence study of isolated minerals from irradiated food. International Symposium on Luminescence Spectrometry (ISLS – 2010), Prague, Czech Republic.

8.   Bhaskar Sanyal, S. P. Chawla, Arun Sharma. (2008). Identification of irradiated potato by thermoluminescence characteristics of isolated minerals. International Food Convention IFCON. 15-19, December. Mysore.

Name	:	**Somnath Ghosh**
Enrolment No.	:	LIFE01200604005
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Radiation Induced Signalling in Mammalian Cells

Abrstract

Ionising radiation leads to a cascade of signaling events which include activation of alarm signals, cytotoxic and cytoprotective signaling pathways, nitric oxide production etc. These events culminate in the death or survival of the irradiated cell. The end result seems to depend upon the pathway predominantly activated. Ionizing radiation has been an important part of cancer treatment for almost a century; radiotherapy is given as fractionated doses ranging from 2-4 Gy, per fraction. The effect of fractionated doses of γ-irradiation (2Gy per fraction over 5 days), as delivered in cancer radiotherapy, was compared with acute doses of 10 and 2Gy, in A549 cells. A549 cells were found to be relatively more radioresistant if the 10Gy dose was delivered as a fractionated regimen. There was intense activation of DNA repair pathway-associated genes (DNA-PK, ATM, Rad52, MLH1 and BRCA1), efficient DNA repair and phospho-p53 was found to be translocated to the nucleus of A549 cells exposed to fractionated irradiation. MCF-7 cells responded differently in fractionated regimen. Silencing of the Rad52 gene in fractionated group of A549 cells made the cells radiosensitive. The above result indicated increased radioresistance in A549 cells due to the activation of Rad52 gene.

Having established that among the different cell lines, A549 was the most radioresistant, the variance in signaling pattern and effectiveness of cell killing with the change in LET was looked at. The survival of the A549 cell line could also be significantly decreased by charged particle irradiation. The mechanism of which seems to be a lack of repair, despite the activation of some of the component of the repair pathway.

Having established that the response of the signaling factors varied with dose, dose fractionation, time, microenvironment and radiation quality (LET), it was of interest to investigate radiation induced bystander signaling. The contribution of the bystander effect to the decrease in survival of A549 cells cannot be ruled out. There was a significant bystander response by unirradiated A549 cells. The mechanism of which may be via NO generation.

Publications

1. Ghosh, S.; Krishna, M. Role of Rad52 in fractionated irradiation induced signaling in A549 lung adenocarcinoma cells. *Mutation Research/Fundamental and Molecular M echanisms of Mutagenesis*; 2012 Jan 3;729(1-2):61-72.

2. Ghosh, S.; Narang, H.; Sarma, A.; Krishna, M. DNA damage response signaling in lung adenocarcinoma A549 cells following gamma and carbon beam irradiation. *Mutation Research/Fundamental and Molecular Mechanisms of Mutagenesis*; 2011 Nov 1;716(1- n 2):10-9.

3. Ghosh, S.; Narang, H.; Sarma, A.; Kaur, H.; Krishna, M. Activation of DNA damage response signaling in lung adenocarcinoma A549 cells following oxygen beam irradiation. *Mutat Res* 723:190-198; 2011.

4. Ghosh, S.; Bhat, N. N.; Santra, S.; Thomas, R. G.; Gupta, S. K.; Choudhury, R. K.; Krishna, M. Low energy proton beam induces efficient cell killing in A549 lung adenocarcinoma cells. *Cancer Invest* 28:615-622; 2010.

5. Ghosh, S.; Maurya, D. K.; Krishna, M. Role of iNOS in bystander signaling between macrophages and lymphoma cells. *Int J Radiat Oncol Biol Phys* 72:1567-1574; 2008. 254

Symposia

1. Ghosh S and Krishna M. Role of Nitric Oxide in Radiation induced Bystander Signaling. Presented at International Conference on Advances in Free Radical Research: Natural products, antioxidant and radioprotector, CSM Medical University, Lucknow. March 19- 21, 2009

2. Ghosh S and Krishna M. Mechanism of relative radioresistance of different cell lines. Presented at DAE-BRNS 4th Life Science Symposium on Recent Advances in mmunomodulation in Stress and Cancer, BARC, Mumbai. December 22-24, 2008

3. Ghosh S and Krishna M. Radiation Induced Bystander Effect: Similar and dissimilar cells. Presented at International Conference on Free Radical & Natural Products in Health, University of Rajasthan, Jaipur, 14-16th February, 2008.

4. Ghosh S, Maurya DK and Krishna M. Molecular Mechanism of Bystander effect insimilar cells: Lack of Bystander effect in dissimilar cells. Presented at DAE-BRNS Symposium 2007 on DNA damage, Repair and their Implications, BARC, Mumbai, 5-7, December, 2007.

Name	:	**Ramanjaneyulu**
Enrolment No.	:	CHEM01200604020
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Chemical Characterization of Nuclear Materials for Trace Elements

Abrstract

Determination of trace elements is important and required for many applications in nuclear technology, for example, the chemical characterization of different materials with respect to trace elements is a necessary quality assurance step. Critical trace constituents like boron which has high thermal neutron absorption cross section, need to be determined with the highest possible precision and accuracy for a rigorous quality assurance in front end nuclear fuel cycle. In back end fuel cycle, ^{137}Cs which will be present in all nuclear waste streams has to be determined before its disposal or vetrification due to its health hazardousness and its long half life & high thermal out put respectively. Even though there are analytical techniques available for this purpose, but there is enough scope to develop new alternative methodologies or further improvement in the existing methodology. The highlights of the present investigations are

1. Three independent methodologies namely chemical prompt gamma neutron activation analsis (CPGNAA), spectrometry and potentiometry with BF_4 ion selective electode have been developed to determine boron in various materials of interest in nuclear technology.

2. For the first time CPNGAA has been employed to determine boron of ppm level even at low neutron fluxes i.e. at 10^6 n/cm^2/Sec.

3. The well known spectrophotometric method for the determination of boron in uranium compounds with curcumin after extraction with 2-ethyl hexane 1 ,3 diol has been modified to allow mg sample size. Investigations were carried out to understand the nitric acid interference in methodology and to circumvent the same. By changing dissolution conditions, this method has been extended to determine boron content in U-Si-Al intermetallic compound, SILUMIN, Al-Si alloy, U_3Si_2 and Zr-Nb alloy samples.

4. For the first time BF_4 ISE has been employed to determine boron in Zr-Nb alloy samples.

5. New ion selective electrodes for Cs$^+$ was developed employing various calyx[4] arene compounds as an ionophores. Employing ion exchange resins in inner filling solutions, response and selectivity for cesium are improved and they are successfully employed to determine Cs$^+$ concentration in simulated high level nuclear waste solutions. The life time of the electrode is 10 months which is longest life time so far reported for any Cs$^+$ ISEs.

    The work describes in the thesis has led to 7 (seven) publications in peer reviewed International Journals.

Publications

1. Determination of boron in water samples by chemical prompt gamma neutron activation analysis, P.S. Ramanjaneyulu, Y.S. Sayi, T. Newton Nathaniel, A.V.R. Reddy and K.L. Ramakumar, *Journal Of Radioanalytical and Nuclear Chemistry*, 273 (2007) 411-414.

2. Determination of boron in uranium compounds by spectrophotometry and studies on effect of HNO3, P.S. Ramanjaneyulu, Y.S. Sayi, V.A. Raman and K.L. Ramakumar, Journal Of Radioanalytical and Nuclear Chemistry, 274 (2007) 109-114.

3. Determination of boron in uranium–aluminum-silicon alloy by spectrophotometry and estimation of expanded uncertainty in measurement, P.S. Ramanjaneyulu, Y.S. Sayi, K.L. Ramakumar, Journal of Nuclear Materials, 378 (2008) 139-143.

4. \Ion selective electrode for Cesium based on 5-(4⬜-nitrophenylazo) 25,27-bis(2-propyloxy) 26,28-dihydroxycalix[4] arene, P.S. Ramanjaneyulu, Parminder Singh, Y.S. Sayi, H.M. Chawla, K.L. Ramakumar, Journal of Hazardous Materials, 175 (2010) 1031-1036.

5. Estimation of Uncertainty in Measurement of Boron in Zr-Nb Alloy Samples by BF4 - Ion Selective Electrode, P.S. Ramanjaneyulu, K.L. Ramakumar and Y.S. Sayi, Accrediation and Quality Assurance journal 15 (2010) 665-671. 127

6. Determination of boron in Zirconium – Niobium alloys by spectrophotometry, P.S. Ramanjaneyulu, Y.S. Sayi and K.L. Ramakumar, Indian Journal of Chemical Technology 17 (2010) 468-470.

7. A new Ion selective electrode for Cesium based on calix[4]arene crown-6compounds. P.S. Ramanjaneyulu, AbhaNaveen Kumar, Y.S. Sayi, K.L. Ramakumar, S.K. Nayak and S. Chattopadhyay, Journal of Hazardous Materials, 205-206 (2012) 81-88.

Technical Reports

1. Determination of Boron in Zirconium – Niobium Alloys by Spectrophotometry and BF4 ISE - Estimation of Expanded Uncertainty in Measurements, P.S. Ramanjaneyulu, Y.S. Sayi, K.L. Ramakumar, B.A.R.C. Report No., BARC/2009/R/003.

Conferences

1. Determination of Boron in Silicon Related Nuclear Materials by Spectrophotometry P.S. Ramanjaneyulu, Y.S. Sayi and K.L. Ramakumar Page No.477, Nuclear and Radiochemistry Symposium (NUCAR-07), Feb14-17, 2009. MS University, Vadodara, India

2. Determination of Boron in Zirconium – Niobium Alloys Spectrophotometry and BF4 - ISE, P.S. Ramanjaneyulu, Y.S. Sayi and K.L. Ramakumar, Page no. 465, Nuclear and Radiochemistry Symposium (NUCAR-09), Jan 7-10, 2009.SVKM Mithibai College, Vile Parle, Mumbai.(Oral Presentation) 128

3. Development of Ion Selective Electrode for Cesium., P.S. Ramanjaneyulu, Anil Boda, Y.S. sayi, K.L. Ramakumar, Parminder Singh, H.M. Chawla and K.L. Ramakumar, Page no. 461, Nuclear and Radiochemistry Symposium (NUCAR-09), Jan 7-10, 2009. SVKM Mithibai College, Vile Parle, Mumbai.

4. Development new ion selective electrode for cesium, P.S. Ramanjaneyulu, AbhaNaveen Kumar, Y.S. Sayi, K.L. Ramakumar, S.K. Nayak andS. Chattopadhyay, Page No.483, Nuclear and Radiochemistry Symposium (NUCAR-11), Feb 22-25, 2011, GITAM University, Visakhapatnam, India.

Name	:	**Geevarghese Philip**
Enrolment No.	:	MATH10200605007
Constituent Institute	:	Institute of Mathematical Sciences, Chennai
Title	:	The Kernelization Complexity of Some Domination and Covering Problems

Abrstract

In a graph *domination* problem the input is a graph, and the question is whether there exists a subgraph which "dominates" the rest of the graph. For example, in the archetypal Dominating Set problem the input consists of a graph G and a positive integer k, and the question is whether there exists a set S of at most k vertices of G such that there is an edge in the graph from every vertex not in S to some vertex in S — such a set S is called a *dominating set* of the graph. Other graph domination problems either put different constraints on the subgraph, or define the notion of domination differently, or both. In a graph *covering* problem the input is again a graph, and the question is whether there exists a subgraph whose removal from the graph results in a "simple" graph.

For example, in the classical Vertex Cover problem the input consists of a graph G and a positive integer k, and the question is whether there exists a set S of at most k vertices of G such that removing S from G leaves a graph with no edges. Other graph covering problems either put different constraints on the subgraph, or define the notion of simplicity differently, or both.

We investigate the *kernelization complexity* of some NP-hard domination and covering problems. Very briefly, the idea is to associate a *parameter* – a positive integer which may be expected to be small for large classes of inputs – with each input instance. The problem now is to see if we can compress the instance in polynomial time to an *equivalent* instance whose size is a small function of the parameter, in polynomial time. Compressing the input to a small size then enables us to apply other methods on the small instance to solve the original problem in feasible time.

In this Thesis we obtain various upper and lower bounds on the kernelization complexity of the following graph domination and covering problems. In each case, the parameter is the size of the solution being sought: Dominating Set, Connected

Dominating Set, Pathwidth-One Vertex Deletion, Connected Feedback Vertex Set, Total Vertex Cover, and Total Edge Cover.

Publications

1. Neeldhara Misra, Geevarghese Philip, Venkatesh Raman, and Saket Saurabh. The effect of girth on the kernelization Complexity of Connected Dominating Set. In Kamal Lodaya and Meena Mahajan, editors, IARCS Annual Conference on Foundations of Software Technology and Theoretical Computer Science, FSTTCS 2010, December 15-18, 2010, Chennai, India, Volume 8 of LIPIcs, Pages 96-107. Schloss Dagstuhl – Leibniz-Zentrum fuer Informatik, 2010.

2. Neeldhara Misra, Geevarghese Philip, Venkatesh Raman, Saket Saurabh, and Somnath Sikdar. FPT Algorithms for Connected Feedback Vertex Set. In Md. Saidur Rahman and Satoshi Fujita, editor WALCOM, volume 5942 of Lecture Notes in Computer Science, Pages 269-280. Springer, 2010.

3.   Neeldhara Misra, Geevarghese Phillip, Venkatesh Raman, Saket Saurabh, and Somnath Sikdar. Fpt algorithms for connected feedback vertex set. Journal of Combinatorial Optimization, Page 1-16, 2011. 10.1007/s10878-011-9394-2.

4.   Geevarghese Philip, Venkatesh Raman, and Somnath Sikdar. Solving Dominating Set in Larger Classes of Graphs: FPT Algorithms and Polynomial Kernels. In Amos Fiat and Peter Sanders, editors, Algorithms – ESA 2009, 17th Annual European Symposium, Copenhagen, Denmark, September 7-9, 2009. Proceedings, volume 5757 of lecture Notes in Computer Science, pages 694-705, 2009.

5.   Geevarghese Philip, Venkatesh Raman, and Yngve Villanger. A Quartic Kernel for Pathwidth-One Vertex Deletion. In Graph Theoretic Concepts in Computer Science – 36th International Workshop, WG 2010, Zaros, Crete, Greece, June 28-30, 2010 Revised Papers, Volume 6410 of Lecture Notes in Computer Science, Page 196-207, 2010.

Name	:	**Amitava Roy**
Enrolment No.	:	PHYS01200704001
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Intense Gigawatt Relativistic Electron Beam Generation Studies in Planar and Cylindrical Diodes

Abrstract

Intense gigawatt relativistic electron beams (IREB) have found applications in the field of high-power microwave generation (HPM), free electron lasers, flash X-ray (FXR) generation, and surface modification etc. For all these applications, the intense electron beam is generated in field emission diode from the explosive emission cathode plasma. When the intense electron beam hits the anode, an anode plasma is produced. Space charge limited electron and ion emission occurs from these electrode plasmas. Movement of electrons, ions, electrode plasmas and the plasma uniformity controls various processes occurring in the high power vacuum diodes. Considerable experimental and theoretical work has been done in the study of beam generation processes but the information available is far from complete. An attempt has been made to understand the beam generation process under various diode configurations and also production of HPM from axial and coaxial virtual cathode oscillator using these beams. KALI 1000 and KALI 5000 (Kilo Ampere Linear Injector) pulse power system has been used to investigate the various aspects of IREB generation. KALI 5000 pulse power system has been operated without a prepulse switch to study the effect of prepulse generated plasma on IREB generation. The typical electron beam parameters studied were 200-450 keV, 10-40 kA, 100 ns with few hundreds of A/cm^2 current density.

Publications

1. Amitava Roy, J. Mondal, R. Menon, S. Mitra, D.D.P.Kumar, Archana Sharma, K.C.MIttal, K.V.Nagesh, D.P.Chakravarthy, "Intense Gigawatt Relativistic Electron Beam Generation in the Presence of Prepulse. Part II," *J. Appl. Phys.*102, 064902 (2007).

2. Amitava Roy , R. Menon, S. Mitra, D. D. P. Kumar, Senthil Kumar, Archana Sharma, K. C. Mittal, K.V. Nagesh, D. P. Chakravarthy, "Intense Relativistic Electron Beam Generation and Prepulse effect in High Power Cylindrical Diode," *J. Appl. Phys.*103, 014905 (2008). This article has been selected for publication on February 2008 issue of VIRTUAL JOURNAL OF ULTRAFAST SCIENCE.

3. Amitava Roy , R. Menon, S. Mitra, D. D. P. Kumar, Senthil Kumar, Archana Sharma, K.C. Mittal, K.V. Nagesh, D. P. Chakravarthy, "Intense Electron Beam Generation in a High Power Cylindrical Diode with a Bipolar Pulse," *J. Appl. Phys.* 103, 096104 (2008).

4. Amitava Roy , R. Menon, S. Mitra, D. D. P. Kumar, Senthil Kumar, Archana Sharma, K. C. Mittal, K.V. Nagesh, D. P. Chakravarthy, "Impedance collapse and beam generation in a high power planar diode," *J. Appl. Phys.* 104, 014904 (2008).

5. Amitava Roy, R. Menon, S. Mitra, D. D. P. Kumar, Senthil Kumar, V. K. Sharma, Ankur Patel, Archana Sharma, K. C. Mittal, K.V. Nagesh, and D. P. Chakravarthy, "Effect of cathode diameter on intense relativistic electron beam generation in the presence of prepulse," *J. Appl. Phys.* 104, 014905 (2008).

6. Amitava Roy, S. Mitra, R. Menon, D. D. P. Kumar, Senthil Kumar, Archana Sharma, K. C. Mittal, K.V. Nagesh, D. P. Chakravarthy, "Prepulse Suppression on a High Power Electron Beam Accelerator using a Dielectric Cathode Holder," *IEEE Trans. Plasma Sci.* Vol. 37, pp. 67-75 (2009).

7. Amitava Roy, S. K. Singh, R. Menon, D. Senthil Kumar, R Venkateswaran, M. R. Kulkarni, P. C. Saroj, K. V. Nagesh, K. C. Mittal, D. P. Chakravarthy, "Measurement of high-power microwave pulse under intense electromagnetic noise," *Pramana – Journal of Physics*, 74, pp. 123-133 (2010).

Name	:	**Sohrab Abbas**
Enrolment No.	:	PHYS01200804001
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Studying Neutron Dynamical Diffraction Theory and its Applications in Neutron Optics

Abrstract

This thesis elucidates intricacies of the dynamical diffraction theory and its applications in design, fabrication and operation of novel neutron optical devices and several experimental firsts scored with these devices. I present the first ever calculations and experimental observations of the deflection $\delta_{cr}(\theta)$ and intensity fraction of neutrons forward diffracted by a single crystal prism as a function of the angle of incidence θ. In the vicinity of a Bragg reflection, $\delta_{cr}(\theta)$ deviates sharply from δ_{am} for an indentical amorphous prism, reaching opposite extrema at either end of the total reflectivity domain and exhibiting a 3 orders of magnitude greater sensitivity to the incidence angle. A nearly plane wave (sub arcsee angular width) neutron beam by employing an optimally designed Bragg prism has been produced, scoring several experimental firsts with it. Analytic expressions for intensity fraction I_H and exit angle θ_H of neutrons diffracted from a Bragg prism are derived. This novel setup has produced a monochromated beam of 0.58 arcsec angular width, which is the best and the tightest neutron collimation achieved to date. This has facilitated SUSANS (Super Ultra-Small-Angle Neutron Scattering) experiments probing wave vector transfers $Q \sim 10^{-6}$ A^{-1} and hence characterization of up to 150 μm-size agglomerates in samples. The transerve coherence length of 175 μm of the monochromated beam is the highest achieved to date, allowing recording of the first neutron diffraction pattern from a macroscopic grating of 200 μm period. Further, I describe a proposal of the high-precision interferometric determination of the coherent scattering length b_c by optimizing various experimental parameters. A finely surfaced thick dual sample in the mondispersive configuration and a large interferometer with spacious splitter-mirror and mirror-analyser gaps operating at a large Bragg angle reduce impreciston in previous b_c measurements down to a few ppm. The correct phase formula by accounting for the refraction effects at the sample-ambient interfaces is derived. The refractive index for neutrons can then be determined to a phenomenal precision of a few parts in 10^{12}. In an interferometric experiment, I have determined b_c of silicon to within 27parts in 10^6, which is $\sim$ twice better to previous measurements by Ioffe'e tal.

Publications

1.   Sohrab Abbas, A.G. Wagh, M Stobl and W Tremier, Nuclear Instruments and Methods in Physics Research A, 634 (2011) S144.

2.   A.G Wagh, Sohrab Abbas and Wolfgang Trimer, Nuclear Instruments and Methods in Physics Research A, 634 (2011) S41.

3.   Sohrab Abbas, Apoorva G. Wagh, Markus Strobl and Wolfgang Treimer, Journal of Physics (CS), 251 (2010) 012073.

4.   Apoorva G. Wagh, Sohrab Abbas and Wolfgang Treimer, Journal of Physics (CS), 251 (2010) 012074.

5.   S. Abbas and A.G. Wagh,Sol.St. Phys. (India) 54 (2009) 463.

6.   Bense Experimental reports 2008 (Helmholtz – zentrum Germany), Apoorva G. Wagh Sohrab Abbas and Wolfgang Treimer

7.   Sohrab Abbas, Apoorva G. Wagh and Wolfgang Treimer, Sol. St. Phys. (India) 53 (2008) 555.

8.   Apoorva G. Wagh, SohrabAbbas, and Wolfgang Triemer, Sol. St. Phys. (India) 53 (2008) 553.

9.   S.Abbas, A.G. Wagh, and W Trimer, Pramana-J. Phys. 71 (2008)1109.

10.   S.Abbas and A.G. Wagh, Pramana-J. Phys. 71 (2008) 1115.

11.   A.G.Wagh, and Abbas abd W Treimer, Pramana –J.Phys 71 (2008) 1171.

12.   A G Wagh, S Abbas & W Trimer, Bensc Experimental reports 2007 (HMI, Germany, 2008) 223.

13.   Sohrab Abbas, Apoorva G. Wagh, Markus Stobl & Wolfgang Treimer, Sol. St. Phys. (India) 52 (2007) 441.

14.   A.G. Wagh, S.Abbas, M. Strobl & W. Treimer, Bensc experimental reports 2006 (HMI, germany, 2007) 22.

15.   M Strobl, W Treimer, Ch Ritzoulis, A.G. Wagh, S. Abbas & I. Manke, J.Apl. Cryst (2007) 40 (supplement) s463

16.   Sohrab Abbas, Aproova G. Wagh, Markus Strobl and Wolfgang Treimer, Abstract book CNSMS (2009) 112

17.   S.Abbas, A.G. Wagh, M. Strobl and W. Treimer, Sol. St. Phys. (India) 51 (2006) 351.

18.   A.G. Wagh, S. Abbas, M.Strobl & W. Treimer, Bensc experimental reports 2005 (HMI Germany, 2006) 115.

19.   A.G. Wagh, and S. Abbas, Sol. St. Phys. (India) 51 (2006) 353

20.   S. Abbas and A.G. Wagh Sol. St. Phys. (India) 50 (2005) 317

21.   A.G. Wagh, and S. Abbas, Sol. St. Phys. (India) 50 (2005) 99

22.   A.G. Wagh and S. Abbas J. Res. Natl. Stad. Technol. 110, 237-240 (2005)

23.   S. Abbas and A.G. Wagh Pramana J-Phys., 63, 375 (2004).

24.   Comment on "Precision Measurement of the n-^{3} He Incoherent Scattering Length Using Neutron Interferometry", Sohrab Abbas and Apoorva G. Wagh Phys.Rev. Lett (accepted)

25.   Sohrab Abbas, Apoorva G. Wagh, and Wolfgang Treimer, Sol. St. Phys. (India) 54 (2009) 212

26.   Sohrab Abbas, Apoorva G. Wagh, R. Loidl, H. Rauch, AIP Conf. Proc. 1349 (2011) 501.

27.   A.G. Wagh, S. Abbas T. Potocar,H. Lemmel, H. Rauch, ILL Experimental reports 3-15-61, 2009 (Grenoble, France, to be Published)

28.   A.G. Wagh, S. Abbas T. Potocar,H. Lemmel, H. Rauch, AIP Conf. Proc., (2011) Accepted Sohrab Abbas, A.G. Wagh, M Stobl and W Tremier, Nuclear Instruments and Methods in Physics Research A, 634 (2011) S144.

29.   A.G Wagh, Sohrab Abbas and Wolfgang Trimer, Nuclear Instruments and Methods in   Physics Research A, 634 (2011) S41.

30.   Sohrab Abbas, Apoorva G. Wagh, Markus Strobl and Wolfgang Treimer, Journal of Physics (CS), 251 (2010) 012073.

31.   Apoorva G. Wagh, Sohrab Abbas and Wolfgang Treimer, Journal of Physics (CS), 251 (2010) 012074.

32.   S. Abbas and A.G. Wagh,Sol.St. Phys. (India) 54 (2009) 463. Bense Experimental reports 2008 (Helmholtz – zentrum Germany), Apoorva G. Wagh Sohrab Abbas and Wolfgang Treimer

33.   Sohrab Abbas, Apoorva G. Wagh and Wolfgang Treimer, Sol. St. Phys. (India) 53 2008) 555.

34.   Apoorva G. Wagh, SohrabAbbas, and Wolfgang Triemer, Sol. St. Phys. (India) 53 (2008) 553.

35.   S.Abbas, A.G. Wagh, and W Trimer, Pramana-J. Phys. 71 (2008)1109.

36.   S.Abbas and A.G. Wagh, Pramana-J. Phys. 71 (2008) 1115.

37.   A.G.Wagh, and Abbas abd W Treimer, Pramana –J.Phys 71 (2008) 1171.

38.   A G Wagh, S Abbas & W Trimer, Bensc Experimental reports 2007 (HMI, Germany, 2008) 223.

39.   Sohrab Abbas, Apoorva G. Wagh, Markus Stobl & Wolfgang Treimer, Sol. St.   Phys. (India) 52 (2007) 441.

40.   A.G. Wagh, S.Abbas, M. Strobl & W. Treimer, Bensc experimental reports 2006   (HMI, germany, 2007) 22. M Strobl, W Treimer, Ch Ritzoulis, A.G. Wagh, S. Abbas & I. Manke, J.Apl. Cryst (2007) 40 (supplement) s463

41.   Sohrab Abbas, Aproova G. Wagh, Markus Strobl and Wolfgang Treimer,   Abstract book CNSMS (2009) 112

42.   .Abbas, A.G. Wagh, M. Strobl and W. Treimer, Sol. St. Phys. (India) 51 (2006) 351.

43.   A.G. Wagh, S. Abbas, M.Strobl & W. Treimer, Bensc experimental reports 2005 (HMI Germany, 2006) 115.

44.   A.G. Wagh, and S. Abbas, Sol. St. Phys. (India) 51 (2006) 353

45.   S. Abbas and A.G. Wagh Sol. St. Phys. (India) 50 (2005)

46.   A.G. Wagh, and S. Abbas, Sol. St. Phys. (India) 50 (2005) 99

47.   A.G. Wagh and S. Abbas J. Res. Natl. Stad. Technol. 110, 237-240 (2005)

48.   S. Abbas and A.G. Wagh Pramana J-Phys., 63, 375 (2004)

49.   Comment on "Precision Measurement of the n-^{3} He Incoherent Scattering   Length Using Neutron Interferometry", Sohrab Abbas and Apoorva G. Wagh Phys.Rev. Lett (accepted)

50.   Sohrab Abbas, Apoorva G. Wagh, and Wolfgang Treimer, Sol. St. Phys.   (India) 54 (2009) 212

51.   Sohrab Abbas, Apoorva G. Wagh, R. Loidl, H. Rauch, AIP Conf. Proc. 1349 (2011) 501.

52.   A.G. Wagh, S. Abbas T. Potocar,H. Lemmel, H. Rauch, ILL Experimental   reports 3-15-61, 2009 (Grenoble, France, to be Published)

53.   A.G. Wagh, S. Abbas T. Potocar,H. Lemmel, H. Rauch, AIP Conf. Proc., 2011) Accepted

Name   :   **Ajit G. Chande**
Enrolment No.   :   LIFE09200604011
Constituent Institute   :   Tata Memorial Centre, Mumbai   :
Title   :   Use of Lentiviral Vector for Improved System of Protein
                                            Expression in Mammalian Cells

Abrstract

Lentiviral vectors can efficiently deliver genetic payloads, making it possible to deliver expression cassettes that direct long term expression of recombinant transgene products, in broad range of cell types. The present dissertation reports development and efficacy validation of HIV-2 derived multiple differently configured transfer vectors with expanded utility for *in vitro* and *in vivo* transgenesis. Among the features imparted, the new ones include a blue/white colony screening platform, a reduced vector backbone and availability of default dual tags for functional proteomics studies. Simultaneously, panels with different utilities were also made these include neomycin or puromycin selection markers, with options of default promoter and availability of dual multiple cloning site (MCS). Each transfer vector format was tested by appropriate transgene expression function by transduction of target cells. During lentiviral transgene delivery, only the cells that are transduced by the vector receive the effect of the transgene coded recombinant protein. To bypass this limitation, we report a novel strategy to amplify the effect of the lentivirally delivered gene product in bystander cells. In this vector system the transgene coded protein is secreted with a cell penetrating peptide (CPP) allowing entry of the same to nearby untransduced bystander cells resulting effectively in an increased biodistribution of the delivered gene product. The efficacy of the enhanced biodistribution system was tested *in vitro* and *in vivo* using GFP as a transgene product and protein transfer to neighboring untransduced cells was observed when green fluorescent protein (GFP) was secreted with a CPP tag. This novel lentiviral vector platform can thus be used to effectively deliver recombinant proteins with enhanced bioavailability into the target organ for desired effect. Furthermore, LV platform was also effectively used for the development of novel reporter cell based antiviral screening assay for rapid evaluation of Tat-TAR interaction inhibitors. The system was validated by establishing a stable cell line and treating with *tat* targated shRNA and a small molecule inhibitor K37 *in vitro*. This is the simplest assay developed so far requiring test material addition as the only manipulation for screening of putative Tat-TAR antagonists for adjunct AIDS therapy. Utility of this vector system was further expanded to device a mammalian expression system for the production of therapeutic recombinant human erythropoietin (rhEPO) in serum free medium.

The expanded configurations of this indigenously developed LV will significantly aid in preferential applications and thus increase its utility as a versatile system for gene transfer technology. Appropriate vector formatting with methods of cell type specific gene delivery will further assist in better gene therapy strategy evaluation using Lentiviral vectors.

Publications

1.   A Single Step Assay for Rapid Evaluation of Inhibitors Targeting HIV Type 1 Tat-MediatedLong Terminal Repeat Transactivation. Ajit G. Chande, Masanori Baba, and Robin Mukhopadhyaya, AIDS RESEARCH AND HUMAN RETROVIRUSES.Volume 27, Number 00, 2011ª Mary Ann Liebert, Inc. DOI:10.1089/aid.2011.0228

2.   Uncoupling Protein 2 Negatively Regulates Mitochondrial Reactive Oxygen Species Generation and Induces Phosphatase-Mediated Anti-Inflammatory Response in Experimental Visceral Leishmaniasis, Writoban Basu Ball, Susanta Kar, Madhuchhanda Mukherjee, Ajit G. Chande, Robin Mukhopadhyaya, and Pijush K. Das, The Journal of Immunology

Name   :   **Surajit Panja**
Enrolment No.   :   CHEM01200804014
Constituent Institute   :   Bhabha Atomic Research Centre, Mumbai :
Title   :   Studies on the Transport Behaviour of Actinides and
                                    Lanthanides Across Supported Liquid Membranes Containing
                                    Di-Glycolamide Carriers

Abrstract

The thesis deals with studies on the transport behavior of actinides and lanthanides across supported liquid membranes containing di-glycolamide carriers.

Liquid Membrance Technique is important for remediation of nuclear waste due to various advantages like low ligand inventory, simultaneous extraction and strinpping, low energy consumptions. Novel carrier molecules of di-glycolamide family were evaluated in detail to understand the transport behavior of various actinides in different oxidation states, lanthanides and fission products. The two molecules studied in detail were TODGA (N,N,N'.N'- tetraoctyl diglycolamide), TEHDGA(N,N,N',N'- tetra (2-ethyl hexyl) diglycolamide.

Different parameters that control the permeation rate were tested to achieve optimum transport rate for TODGA as carrier for the different actinides viz, Pu(III,IV), U(VI),Th(IV). Effect of diluents on the extractability and transport rate of Am(III) for TODGA as extractant/carrier was also studied as phase modifier and radiation induced degradation of the TODGA-DHOA solvent system on the transport of different actinides and fission product was also investigated in detail.

A Branched chain analog of TODGA, TEHDGA was also used to study the transport behavior of Am(III), Eu(III) and U(VI) from nitric acid medium. Effective transport for all the radio-nuclides was observed after optimizing various parameters. Stability of the membrane was also found to be reasonable over the period of time studied.

A series of substituted di-glycolamides were studied in detail to understand their behavior for the solvent extraction and liquid membrane transport behavior of A(III) and Sr(II). Different parameters were investigated and decontamination factor of Am(III) over Sr(II) were evaluated. Optimum molecule with respect to extractability and D.F was found to be TODGA.

The work described in the thesis has led to 11 (eleven) publications in peer reviewed International Journals.

Publications

1. Facilitated Transport of Am(III) through a Flat Sheet Supported Liquid Membrane(FSSLM) containing Tetra (2-Ethyl) Hexyl Diglycolamide (TEHDGA) as carrier; S.Panja, R.Ruhela, S.K.Misra, J.N.Sharma, S.C.Tripathi, A.D.Moorthy, *J. of Membr. Sci.,* 325 (2008) 158–165.

2. Studies on uranium(VI) pertraction across a N,N,N',N'-tetraoctyldiglycolamide (TODGA) supported liquid membrane, S. Panja, P.K. Mohapatra, S.C.Tripathi,V.K. Manchanda, *J. of Memb. Sci.,* 337 (2009) 274–281.

3. Transport of Thorium(IV) Across a Supported Liquid Membrane Containing N,N,N',N'-Tetraoctyl-3-oxapentanediamide (TODGA) as the Extractant, S. Panja, P.K. Mohapatra, S.C. Tripathi, V.K. Manchanda, *Sep. Sci. and Technol.,* 45 (2010)1112-1120.

4. Pertraction of plutonium in the +4 oxidation state through a supported liquid membrane containing TODGA as the carrier, S. Panja, P.K. Mohapatra, P. Kandwal, S.C. Tripathi, V.K. Manchand, *Desalination,* 262 (2010) 57–63.

5. Controlled Pertraction of Plutonium(III) Under Reducing Conditions From Acidic Feeds Using TODGA as the Carrier Extractant, S. Panja, P.K. Mohapatra, S.C. Tripathi, V.K. Manchanda, *Sep. Sci. and Technol.,* 46 (2011)94–104. 302

6. Carrier Facilitated Transport of Europium(III) Across Supported Liquid Membranes Containing N,N,N',N'-tetra-2-ethylhexyl-3-pentanediamide (T2EHDGA) as the Extractant, S. Panja, P.K. Mohapatra, S.K.Misra, S.C. Tripathi, *Sep. Sci. and Technol.,* 46(12)(2011)1941-1949.

7. Facilitated transport of uranium(VI) across supported liquid membranes containing T2EHDGA as the carrier extractant; S. Panja, P.K. Mohapatra, S.C. Tripathi, V.K. Manchanda, *J. of Haz. Mater.,* 188 (2011) 281–287.

8. Permeation of Uranium(VI) Across Supported Liquid Membranes (SLM) Containing T2EHDGA as the Carrier Extractant, S.Panja, P.K. Mohapatra, S.C. Tripathi and V.K. Manchanda, *Desal. & Water Treatment* 38 (2012) 2017-214.

9. Uranium(VI) pertraction across a supported liquid membrane containing a branched diglycolamide carrier extractant: Mass transfer modeling, S.Panja, P.K.Mohapatra, P.Kandwal and S.C.Tripathi, *Desalination* 385(2012)213-218.

10. Role of organic diluents on Am(III) extraction and transport behaviour using N,N,N'N'-tetraoctyl-3-oxapentanediamide as the extractant, S.Panja, P.K. Mohapatra, S.C. Tripathi, P.M.Gandhi and P.Janardan, Journal of Membrane Science, 403-404(2012) 71-77 303

11. Liquid- liquid extraction and pertraction behavior of Am(III) and Sr(II) with diglycolamide carrier extractants, S.Panja, P.K. Mohapatra, S.C. Tripathi,

12. G.D.Dekahne,P.M.Gandhi and P.Janardan, *Journal of Membrane Sci*ence ,399-400(2012) 28-36.

13. Effect of gamma-irradiation of TODGA on the SLM transport behaviour of radio nuclides, S.Panja, P.K.Mohapatra, S.C.Tripathi and P.M.Gandhi (Communicated).

14. Solvent Extraction and liquid membrane studies of Eu(III) using substituted di-glycolamide carrier extractants, S.Panja, P.K. Mohapatra, S.C. Tripathi, G.D.Dekahne and P.M.Gandhi (Communicated)

Conference / Symposia

1. Transport of Am3+ Using Supported Liquid Membrane Containing N,N,N',N'-Tetraoctyldiglycolamide (TODGA) as the carrier; S. Panja, P.K. Mohapatra, A. Dakshinamoorthy, S.K. Munshi, P.K. Dey and V.K. Manchanda, Indian Council Of Chemists, 26th Annual Conf. of the Indian Council of Chemists, Dr.Hari Singh Gaur University, Sagar (M.P.) 26th – 28th February, 2008.

2. Optimization and Stability Studies on Plutonium(III) Transport in Supported Liquid Membranes Containing TODGA as the Carrier Extractant; S. Panja, 304 P.K. Mohapatra, A. Dakshinamoorthy, S.K. Munshi, P.K. Dey and V.K. Manchanda, 333-334, *In proceedings of DAE-BRNS Theme meeting on Emerging Trends in Separation Science and Technology (SESTEC-2008), March 14-18, 2008,* University of Delhi, Delhi.

3. Transport of Thorium(IV) and Uranium (VI) in Supported Liquid Membranes Containing TODGA as the Carrier Extractant; S. Panja, P.K. Mohapatra, A. Dakshinamoorthy, S.K. Munshi, P.K. Dey and V.K. Manchanda, 335-336, *In proceedings of DAE-BRNS Theme meeting on Emerging Trends in Separation Science and Technology (SESTEC-2008), March 14-18, 2008,* University of Delhi, Delhi.

4. Carrier Mediated Transport of Actinide Ions Using Supported Liquid Membranes Containing TODGA as the Carrier Extractant; S. Panja, P.K. Mohapatra, A. Dakshinamoorthy, S.K. Munshi, P.K. Dey and V.K. Manchanda, *18th International Solvent Extraction Conference, ISEC-2008,* Tucson, Arizona, September 15 to 19, 2008 .

5. Effect of gamma-irradiation of TODGA on the SLM transport behaviour of radio nuclides, S. Panja, P.K. Mohapatra, S.C.Tripathi, S.K. Munshi, P.K. Dey and V.K. Manchanda, *In Proceedings of DAE-BRNS Symposium on Nuclear and Radiochemistry (NUCAR-2009)*, held at Bhabha Atomic Research Centre, Mumbai.

6. Transport of uranium(VI) complexes through supported liquid membranes containing N,N,N'N'-tetraoctyl diglycolamide as the carrier extractant; S. 305, Panja, P.K. Mohapatra, S.C. Tripathi, S.K. Munshi, P.K. Dey and V.K. Manchanda, *In Proceedings of DAE-BRNS Symposium on Nuclear and Radiochemistry (NUCAR-2009)*, held at Bhabha Atomic Research Centre, Mumbai.

7. Effect of organic diluents on the transport of Am(III) across TODGA based supported liquid membranes; S. Panja, P.K. Mohapatra, S.C. Tripathi, S.K. Munshi, P.K. Dey and V.K. Manchanda, *Indian Analytical Science Congress 2009,* Lonavala, Maharashtra.

8. Fcilitated transport of U(VI) across a supported liquid membrane(SLM) containing TEHDGA as carrier; S.Panja, P.K.Mohapatra, S.C.Tripathi, S.K.Munshi,P.K.Dey,V.K.Manchanda, *In proceedings of DAE-BRNS Theme meeting on Emerging Trends in Separation Science and Technology (SESTEC-2010)* held at Bhabha Atomic Research Centre.

9. Transport studies of Eu(III) across a Supported Liquid Membrane(SLM) using TEHDGA as carrier; S. Panja, S.K.Misra, P.K. Mohapatra, S.C. Tripathi, S.K. Munshi, P.K. Dey and V.K. Manchanda, *In proceedings of DAE-BRNS Theme meeting on Emerging Trends in Separation Science and Technology (SESTEC-2010)* held at Bhabha Atomic Research Centre.

Name   :   **Sandeep Verma**
Enrolment No.   :   CHEM01200604008
Constituent Institute   :   Bhabha Atomic Research Centre, Mumbai :
Title   :   Ultrafast Electron Transfer Dynamics in Dye-Sensitized
                                      Semiconductor Nano-Materials

Abrstract

This thesis deals with interfacial electron transfer (IET) reactions between molecular adsorbate and wide bandgap semiconductor nanomaterial. It offers an understanding of various molecular level schemes that can be used for the enhancement of the optical response of different dye molecules and for increasing the interfacial charge separation on nanoparticle surface. The semiconductor nanomaterials, notably TiO_2, ZrO_2 nanoparticles (NPs) and ZnO quantum dot (QD) are synthesized and used in the study. Catechol or carboxylate moiety on the dye molecules is used as surface linkage to metal oxide semiconductor nanomaterials.

Beginning with M(II)-polypyridy I complexes (M = Ru or Os), the thesis describes the basics of molecular photophusics and spectral sensitization of TiO_2 NPs. The spectroscopic observables of femtosecond time-resolved transient absorption and picoseconds time-resolved transient emission study are used in assignment of different transient species generated in the IET process. The intermediacy of surface states (TiO_2 NPs), thermalized and non-thermalized excited states (dye), the effects of heavy mental ions (Ru^{II} versus Os^{II}) and electron donating ligand (aminoderivative) are described in the dynamics studies of IET reactions in the thesis.

The thesis elaborates the antenna effects of energy and electron transfer by gradually shifting the IET studies from monomer sensitizer molecules to supramolecular assemblage. Using synthetic porphyrin-aggregates, natural light harvesting pigments-"phycocyanin-allophycocyanin" and polynnuclar-M(II)-polyprideyl-complexes, different models of energy transfer which include exciton, dipole-dipole and super-exchange interactions, are briefly describes in the thesis. The sequential energy transfer pathways of antenna complex sensitized TiO_2 NP or ZnO QD systems are describes in the IET studies. The thesis avails information about how the IET reactions change after inclusion of smaller photosensitizing molecules into larger synthetic- or self-assembly.

The thesis describes the feasibility of newer sensitizer molecules in primary phoroconversion processes. It elucidates various sensitization schemes in fulfillment of large spectral response and improved interfacial charge separation in the dye/semiconductor systems.

Publications

1. Interfacial Electron-Tranfer Dynamics on TiO_2 and ZrO_2 Nanoparticle Surface Sensitized by New Catechol Derivatives of Os(II)-polypyridyl Complexes: Monitoring by Charge-Transfer Emission.Sandeep Verma, Prasenjit Kar, Amitava Das, Dipak K. Palit, Hirendra N. GhoshJ.Phys. Chem.c 2008, 112, 2918.

2. Ultrafast Exciton Dynamics of J- and H-Aggregates of the Porphyrin-Catechol in Aqueous Solution.Sandeep Verma and Hirendra N. GhoshUltrafast Phenomena, Chem. Phys., Springer, 2008,328.

3. Ultrafast Exciton dynamics of J- and H-Aggregates of the Porphyrin-Catechol in Aqueous Solution. Sandeep Verma, Amrita Ghosh, Amitava Das, Hirendra Nath Ghosh.J. Phys. Chem. B 2010, 114, 8327

4. The Effect of Heavy Atoms on Photoinduced Electron Injection from Nonthermalized and Thermalized Donor States of M(II)-Polypyridyl (M=Ru/Os) Complexes to Nanoparticulate TiO_2 Surface: An Ultrafast Time-Resolved Absorption Study.Sandeep Verma, Prasenjit Kar, Amitava Das, Dipak K. Palit, Hirendra N. Ghosh Chem.Eur.J.2010, 16, 611.

5. Efficient Charge Separation in TiO_2 Films Sensitized with Ruthenium (II)- Polypyridyl Complexes: Hole Stabilization by Ligand-Localized Charge-Transfer States. Sandeep Verma, Prasenjit Kar, Amitava Das, Hirendra N. Ghosh Chem. Eur. J. 2011, 17, 1561

6. Exciton-Coupled Charge-Transfer Dynamics in a Porphyrin J-Aggregate/TiO_2 Complex,Sandeep Verma, Amrita Ghosh, Amitava Das, Hirendra Nath Ghosh Chem.Eur.J.2011, 17, 3458

7. Employing a Photosynthetic Antenna Complex to Interfacial Electron Transfer on ZnO Quantum Dot. Sandeep Verma, Alka Gupta, Jayashree K. Sainis, and Hirendra Ghosh J. Phys. Chem. Lett. 2011, 2, 858.

8. Photophysical Study of Ligand Localized Excited State in Ruthenium (II) Polypyridyl Complexes:A Combined Effect of Electron Donor-Acceptor Ligand.Sandeep Verma, Prasenjit Kar, Amitava Das, Hirendra N. GhoshDalton Trans., 2011, 40, 9765.

9. Sequential Energy and Electron Transfer in Polynuclear Complex Sensitized TiO_2 Nanoparticle.Sandeep Verma, Prasenjit Kar, Amitava Das, Hirendra N. Ghosh.J. Phys. Chem. Lett., 2012 (Accepted; dx.doi.org/10.1021/jz3005305).

10. Exciton Energy and Charge Transfer in Porphyrin Aggregate / Semiconductor (TiO_2) Composites.Sandeep Verma and Hirendra N. Ghosh.J. Phys. Chem. Lett. (Perspective), 2012 (Submitted by Invitation)

Name	:	**Vishnu Kumar Sharma**
Enrolment No.	:	PHYS03200704003
Constituent Institute	:	Raja Ramanna Centre for Advanced Technology, Indore:
Title	:	Study of the Magneto-Structural Transition and Associated
		Functional Properties in the Ni-Mn-In and Ni-Mn-Sn Alloys

Abrstract

Our investigations concern various aspects of the SU(2) canonical formulation of gravity.

As is well known, the very basis of the Loop Quantization programme is the real SU(2)formulation of gravity. This framework contains a free parameter, namely, the Barbero-Immirzi parameter ($\eta^{\boxed{}}1$ in our notation). In the corresponding Lagrangian descriptionbased on the Holst action, η appears as a coefficient of the Holst term. This additionalterm and hence η, does not a_ect the classical equations of motion of the Hilbert-Palatini action. However, introduction of matter-coupling in the Lagrangian requiresadditional modifications other than the Holst term in order to preserve the classicalequations of motion. These modifications are not universal and change with the mattercontent of the theory. In [2] we develop a canonical formulation based on an actioncontaining the Nieh-Yan topological density instead of the Holst term. This has thefollowing advantages:

(a) While the new Lagrangian density leads to a real SU(2) theory of gravity as ear-lier, inclusion of matter now does not need any further modifcations and the equations of motion continue to be independent of _ for all couplings (the Nieh-Yan invariant being `universal' in this sense);
(b) The Nieh-Yan term provides a topological interpretation for η unlike the Holst term.

For these reasons, addition of the Nieh-Yan density in the gravity action supercedesthe Holst formulation. As an elucidation of these facts, the method has been applied to spin-1/2 fermions coupled to gravity in [2]. In [3], we perform a similar analysis for spin-3/2 fermions and illustrate how the supergravity theories (N = 1; 2; 4 etc.) in general can be handled likewise.

In four-dimensional gravity, there are two more topological densities other than theNieh-Yan term, namely, the Euler and Pontryagin densities. In a complete theory of gravity, one needs to include all of them. We study the canonical formulation corre- sponding to such a general theory.q

Finally, we investigate what is a suitable quantum framework if the Barbero-immirzi parameter has to emerge as a vacuum angle as the theta parameter in gauge theories. We demonstrate that the standard quantization procedure cannot be used for such a purpose and one needs to adopt alternative quantization procedures, e.g. the Gupta- Bleuler and coherent state quantization.

Publications

1. The effect of external pressure on the magnetocaloric effect of Ni–Mn–In alloy. *J. Phys.: Condens. Matter* 23, 366001 (2011). Sharma V. K., Chattopadhyay M. K. and Roy S. B.

2. Elevating the temperature regime of the large magnetocaloric effect in a Ni–Mn–In alloy towards room temperature. *J. Phys. D: Appl. Phys.* 44, 145002 (2011). Sharma V. K., Chattopadhyay M. K., Sharathchandra L. S., and Roy S. B.

3. Martensitic transition near room temperature and the temperature- and magnetic-fieldinduced multifunctional properties of Ni49CuMn34In16 alloy. *Phys. Rev*. B 82, 172411 (2010). Sharma V. K, Chattopadhyay M. K., Khandelwal A., and Roy S. B.

4. The effect of substitution of Mn by Fe and Cr on the martensitic transition in the Ni50Mn34In16 alloy. *J. Phys.: Condens. Matter.* 22, 486007 (2010). Sharma V. K., Chattopadhyay M. K., Nath S. K., Sokhey K. J. S., Kumar R., Tiwari P., and Roy S. B.

5. \Contrasting magnetic behavior of Ni50Mn35In15 and Ni50Mn34.5In15.5 alloys. *J. Appl. Phys*. 108, 073909 (2010). Chattopadhyay M. K., Manekar M. A., Sharma V. K., Arora P., Tiwari P., Tiwari M. K., and Roy S. B.

6. Large magnetocaloric effect in Ni50Mn33.66Cr0.34In16 alloy.*J. Phys. D: Appl. Phys.* 43, 225001 (2010). Sharma V. K., Chattopadhyay M. K., and Roy S. B.

7. Temperature and magnetic field induced strain in Ni50Mn34In16 alloy. *J. Phys. D: Appl. Phys.* 42, 185005 (2009). Sharma V.K., Chattopadhyay M.K., Chouhan A., Roy S.B.

8. A scanning Hall probe imaging study of the field induced martensite-austenite phase transition in Ni50Mn34In16 alloy. *J. Phys.: Condens. Matter*. 22, 016008 (2009). Sharma V.K., Moore J. D., Chattopadhyay M.K., Morrison K., Cohen L. F., and Roy S.B.

9. Thermomagnetic history dependence of magnetocaloric effect in Ni50Mn34In16. *Appl. Phys. Lett.* 92, 022503 (2008).Chattopadhyay M. K., Sharma V.K., and Roy S. B.

10. Studies on the field-induced martensite to austenite phase transition in Ni50Mn34In16. *J. Phys.: Condens. Matter*. 20, 425210 (2008). Sharma V. K., Chattopadhyay M. K., and Roy S. B.

11. Large inverse magnetocaloric effect in Ni50Mn34In16. *J. Phys. D: Appl. Phys.* 40, 1869 (2007).Sharma V. K., Chattopadhyay M. K., and Roy S. B.

12. Kinetic arrest of the first order austenite to martensite phase transition in Ni50Mn34In16: dcmagnetization studies. *Phys. Rev. B* 76, 140401 (2007). Sharma V. K., Chattopadhyay M. K., and Roy S. B.

13. Magnetocaloric effect in Heusler alloys Ni50Mn34In16 and Ni50Mn34Sn16. *J. Phys.: Condens. Matter* 19, 496207 (2007). Sharma V. K., Chattopadhyay M. K., Kumar R., Ganguli T., Tiwari P., and Roy S. B.

14. Large magnetoresistance in Ni50Mn34In16 alloy. *Appl. Phys. Lett.* 89, 222509 (2006).

15. Sharma V. K., Chattopadhyay M. K., Shaeb K. H. B., Chouhan A., and Roy S. B.

Publications in conferences:

1. Large magnetocaloric effect in Ni50Mn33.66Cr0.34In16 alloy. Proceedings of the DAE Solid State Physics Symposium, Vol. 54, 1017 (2009). Sharma V. K., Chattopadhyay M. K., Kumar R., and Roy S. B.

2. Thermomagnetic history dependence of magnetic field induced strain in Ni50Mn34In16. Proceedings of the DAE Solid State Physics Symposium, Vol. 54 , 1015 (2009). Sharma V.K., Chattopadhyay M.K., and Chouhan A.

3. Study of magnetization and Magnetoresistance across the field induced martensite to austenite transition in Ni50Mn34In16 . Proceedings of the DAE Solid state physics symposium , Vol. 53, 1101 (2008). Sharma V.K., Chattopadhyay M.K., and Roy S.B.

4. Field induced martensite to austenite transition in Ni50Mn34In16 alloy. Proceedings of the DAE Solid State Physics Symposium, Vol. 52 , 1035 (2007). Sharma V.K., Chattopadhyay M.K., Chouhan A., Arora P., and Roy S.B.

5. Effect of annealing on the martensitic transition in Ni50Mn34In16 alloy., Proceedings of the DAE Solid State Physics Symposium, Vol. 52 , 1031(2007). Sharma V.K., Chattopadhyay M.K., Chouhan A., Arora P., Kumar R., Ganguli T., and Roy S.B.

Name	:	**Sandipan Sengupta**
Enrolment No.	:	PHYS10200604014
Constituent Institute	:	Institute of Mathematical Sciences, Chennai
Title	:	Guage Theory of Gravity with Topological Invariants

Abrstract

In gravity theory in four dimensions, there are three possible topological terms which can be added to the Lagrangian density. These are the Nieh-Yan, Pontryagin and Euler terms. Here we investigate the e_ect of these terms in the context of canonical SU(2) formulation of gravity. We set up a general SU(2) formulation for gravity including all three terms. The theory contains three topological parameters associated with the three terms. Finally, we study what could be a suitable quantum framework for gravity in which one of these parameters, namely the Barbero-Immirzi parameter, can be interpreted as a vacuum angle exactly like the theta parameter in gauge theories.

Publications

1. 'Topological interpretation of Barbero-Immirzi parameter' ; G. Date, R. K. Kaul, S. Sengupta; Phys. Rev. D 79, 044008 (2009)

2. `Canonical supergravity with Barbero-Immirzi parameter'; S. Sengupta, R. K. Kaul; Phys. Rev. D 81, 024024 (2010)

3. `Quantum realizations of Hilbert-Palatini second-class constraints'; S. Sengupta; Class. Quantum Grav. 27, 145008 (2010)

4. `Topological parameters in gravity'; R. K. Kaul, S. Sengupta; Phys. Rev. D 85, 024026 (2012)

Name   :   **Sangita Dhara Lenka**
Enrolment No.   :   CHEM01200604029
Constituent Institute   :   Bhabha Atomic Research Centre, Mumbai
Title   :   Analytical Characterization of Technologically Important
                                Materials using TXRF and EDXRF

Abstract

The thesis deals with the studies on the applications of Total Reflection X-ray Fluorescence (TXRF) and Energy dispersive X-ray Fluorescence (EDXRF) for the characterization of technologically important materials.

The TXRF method developed for the trace metal determinations in thorium oxide during participation in an Interlaboratory Comparison Experiment (ILCE) conducted by the Department of Atomic Energy (DAE) for the development of thorium oxide standards for trace metallic impurities, showed that the TXRF results agreed well with the other laboratory results based on the well established methods of trace metals analyses i.e. AAS, ICP-AES, ICP-MS. Hence, the TXRF determined values helped in the certification of seven trace metallic elements in thorium oxide standards. This type of the study using TXRF was done for the first time and established TXRF as an alternative method for the determination of trace elements on routine basis. A TXRF method for the determination of low Z elements (Na, Mg and Al) in uranium matrix was also developed. This method required separation of major matrix and a vacuum chamber for the determination of low Z elements.

TXRF methods for the determination of non-metals such as sulphur and chlorine in nuclear materials were developed successfully. For chlorine determination a pyrohydrolysis hyphenated TXRF method was developed for separation and determination, respectively. The conventional method of pyrohydrolysis was slightly modified to avoid chlorine loss during the TXRF sample preparation. The effect of He purging on the TXRF analysis was also studied and such gas purged TXRF studies were carried out for the first time. Another novel TXRF method for chlorine determination, in acidic medium, was developed.

The microanalytical capability of TXRF was studied for the bulk determination of uranium and thorium in the presence of each other in solution. It was observed that when the sample amount was varied from 30 ng to 12 µg (upto 3 orders of magnitude) on the sample support, the TXRF condition was satisfied. A novel TXRF method for

analyzing solid samples was developed. This method did not require cumbersome dissolution process prior to the analysis. The samples in the form of pellets were gently rubbed on the sample support in such a way that a few ng of the sample was transferred to the sample support. The TXRF spectrum of this specimen was directly measured in the spectrometer. Such analyses give relative amount ratio which can be very useful for the fast and verification of composition in $(U, Th)O_2$ pellets during the fuel fabrication stage.

Apart from the characterization of nuclear materials using TXRF another interesting work on determination of uranium in non-conventional sources such as seawater and fertilizers were carried out.

A novel EDXRF methodology was developed for the fast and accurate determination of uranium and thorium. The method required very less sample amount as only a few micrograms of the sample was

loaded on a filter paper. Such method of analysis can be used to analyse radioactive samples by sealing the sample and hence enclosing of the instrument in the glove box can be avoided. An EDXR

Fmethodology was developed for the determination cadmium at trace levels in uranium using continuum excitation and Mo filter. The work reported in the thesis has led to the development of several new methodologies using TXRF and EDXRF for the characterization of nuclear materials which are technologically important materials. The work described in the thesis resulted in *10 (Ten)* peer reviewed *International Journal* publications.

Publications

1. *Uanium determination in seawater by total reflection X-ray, fluorescence spectrometry, N.L. Misra , *S. Dhara*, K.D. Singh Mudher, Spectrochimica Acta Part B, 61 (2006) 1166–1169

2. *Bulk determination of uranium and thorium in presence of each other by Total Reflection X-ray Fluorescence spectrometry, *Sangita Dhara*, Nand Lal Misra, KhushmDev Singh Mudher, Suresh Kumar Aggarwal, Spectrochimica Acta Part B, 62 (2007) 82–85.

3. *Trace element determination in thorium oxide using total reflection X-ray fluorescence spectrometry , N.L. Misra , *Sangita Dhara*, V.C. Adya , S.V. Godbole, K.D. Singh Mudhera, S.K. Aggarwal Spectrochimica Acta Part B, 63 (2008) 81–85.

4. *Determination of sulphur in uranium matrix by total reflection X-ray fluorescence spectrometry, *Sangita Dhara*, N.L. Misra and S.K. Aggarwal, Spectrochimica Acta Part B, 63 (2008) 1395-1398.

5. *An EDXRF method for determination of uranium and thorium in AHWR fuel after dissolution, *Sangita Dhara*, S. Sanjay Kumar, N.L. Misra and Suresh K. Aggarwal, Xray Spectrometry, 38 (2009) 112-116.

6. *A novel approach for chlorine determination in acidic medium by total reflection X-ray fluorescence, N.L. Misra, Imre Varga, *Sangita Dhara* and S.K. Aggarwal, X-ray Spectrometry, 38 (2009) 182-185.

7. Forensic application of total reflection X-ray fluorescence spectrometry for elemental characterization of ink samples, *Sangita Dhara*, N.L. Misra, S.D. Maind, Sanjukta A. Kumar, N. Chattopadhyay, S.K. Aggarwal, Spectrochimica Acta Part B, 65 (2010) 167– 170.

8. *Determination of low atomic number elements at trace levels in uranium matrix using vacuum chamber total reflection X-ray fluorescence, N.L. Misra, *Sangita Dhara*, M. Óvári, Gy. Záray, S.K. Aggarwal, Imre Varga, Spectrochimica Acta Part B, 65 (2010) 457–460.

9. *Energy dispersive X-ray fluorescence determination of cadmium in uranium matrix using Cd Kα line excited by continuum, *Sangita Dhara*, N.L. Misra, S.K. Aggarwal, V.Venugopal, Spectrochimica Acta Part B, 65 (2010) 461-465.

10. Energy Dispersive X-Ray Fluorescence Determination of Thorium in Phosphoric Acid Solutions, N.N. Mirashi, *Sangita Dhara*, S. Sanjay Kumar, Satyajeet Chaudhury, N.L.Misra, and S.K. Aggarwal, Spectrochimica Acta Part B, 65(2010) 461-465.

11. *Trace Determination of Uranium in Fertilizer Samples by TXRF, N.L. Misra, *Sangita Dhara*, Arijeet Das, G.S. Lodha, S.K. Aggarwal, and I. Varga, PRAMANA- Journal of Physics 76(2011) 357-360.

12. Application of Total Reflection X-ray Fluorescence Spectrometry for Interlaboratory Study for Development of Rainwater Standard, *Sangita Dhara* and *N.L. Misra*, PRAMANA- Journal of Physics 76(2011) 361-366.

Name	:	**Jampa Maruthi Pradeep Kanth**
Enrolment No.	:	PHYS10200604007
Constituent Institute	:	Institute of Mathematical Sciences, Chennai
Title	:	Molecular Mean Field Theory for Liquid Water and Hydrophobic Force

Abstract

We provide a statistical description of hydrogen-bond fluctuations in liquid water and address the long-distance nature of hydrophobic force and also attempt to provide a consistent picture of its dependence on the size of hydrophobes. Our large-scale molecular dynamics simulations reveal an Nunusually long-distance correlation in 'longitudinal' part of dipolar orientational correlation. It is non-vanishing even at 75 °A and falls-off exponentially with correlation lengths 5.2 °A and 24 °A beyond solvation region [1]. Its long-distance behavior is seen to be predominantly influenced by short-ranged hydrogen-bond interaction and, surprisingly, insensitive to Coulomb interactions. This correlation is shown to give rise to a shape-dependant attraction between two hydrophobic surfaces at large distances of separation and the range of this attractive force is in agreement with experiments [1].

Hydrophobic force between large surfaces is analyzed by envisaging a simple lattice model for water with essential features of hydrogen-bond interaction and investigating the thermodynamic consequences of confining hydrogen-bond fluctuations. The restrictions on network formation, due to charge specificity and steric repulsion experienced by bonding partners, manifest as a global sum rule. An analytical framework, called molecular mean field theory, is developed within which thermodynamic properties are analyzed consistent with the sum rule for water and fluctuation properties are deduced about mean field. Large correlation length for orientational fluctuations is seen to be a consequence of the sum rule in liquid phase and Monte Carlo simulations attest mean field results in this high density regime [2].

Large hydrophobic surfaces confining water in their intervening region spatially restrict the hydrogen-bond fluctuation lengthscales and also, modify orientational fluctuations of interface water. This Casimir-like effect is analyzed within the water model using molecular mean field theory technique and hydrophobic force is shown to arise dominantly due to restriction on hydrogen-bond fluctuations in confined water. Explicit expressions are also deduced for interfacial free energy and transverse density profile. A qualitative distinction in the nature of interaction is made between the case of mesoscopic surfaces and macroscopic surfaces based on dominant under- lying mechanism. In either case, the interaction is largely influenced by the long-range correlations of orientational fluctuations [3].

Publications

1. Jampa Maruthi Pradeep Kanth, Satyavani Vemparala, and Ramesh Anishetty. Long-distance correlations in molecular orientations of liquid water and shape-dependent hydrophobic force. Phys. Rev. E, 81(2):021201, 2010.

2. Jampa Maruthi Pradeep Kanth and Ramesh Anishetty. Molecular mean field theory for liquid water. Physica A, 391:439-455, 2012

3. JampaMaruthi Pradeep Kanth and Ramesh Anishetty. Hydrophobic force a Casimir-like effect due to hydrogen-bond fluctuations. arXiv:1109.2733, 2011.

Name	:	**Subrata Dutta**
Enrolment No.	:	CHEM01200604022
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Studies on the Separation of Carrier Free Y-90 from Sr-90 using Diglycolamide Extractants

Abstract

The thesis gives a comparative account of the solvent extraction, extraction chromatography and flat sheet supported liquid membrane transport behavior of Sr(II) and Y (III) using several diglycolamide extractants with an aim of separating carrier free Y-90 for pharmaceutical applications. The liquid – liquid extraction as well as transport behavior of Sr(II) and Y(III) have been carried out in great detail using TODGA and T2EHDGA as the carrier extractions. In the solvent extractions studies, the nature of the extracted species was determined by slope analysis method and separation factor values were calculated at different acidities. Conditions for efficient extraction and separation of Y(III) from Sr(II) were arrived at and the purity of the Y-90 product from actual mixture containing Sr – 90 and Y – 90 was determined by several techniques. The extraction chromatographic method was also used for efficient separation of Y-90 from Sr-90 by a series of batch and column separation studies. A separation method was developing using a TODGA impregnated extraction chromatographic resin material where 3 M HNO_3 was used for loading and pH 2 and 0.01 METDTA at pH 2 were used for the elution of Sr and Y, respectively. The radiolytic stability of the resin and reusability of column were also investigated. Supported liquid membrane separation method was also investigated using a variety of solvent systems using several diluents.

The thesis gives an insight into the possibility of applying various separation techniques using TODGA and in some cases T2EHDGA as the extractant for the separation of Y – 90 from a mixture of Sr-90 and Y-90. The purity of Y-90 has been evaluated by half-life method and was found to be reasonably good in the solvent extraction as well as extraction chromatographic methods while supported liquid membrane based method was found to be yielding products with significant Sr-90 contamination. It was thus required to couple to another separation technique for obtaining high purity carrier free Y-90 for pharmaceutical applications.

The thesis presents a first of its kind study on the separation of Y-90 and Sr-90 using diglycolamide extractions and is highly relevant from application point of view.

Publications

1. Separation of 90Y from 90Sr by a solvent extraction method using N,N,N_,N_-tetraoctyl diglycolamide (TODGA) as the extractant, S. Dutta, P.K. Mohapatra and V.K. Manchanda. *Appl. Radiat. Isot.,* 69 (2011) 158-162.

2. Preferential extraction of 90Y from 90Sr using N,N,N_,N_-tetra-2-ethylhexyl diglycolamide (T2EHDGA) as the extractant, S. Dutta, P.K. Mohapatra, D.R. Raut and V.K. Manchanda. *J. Radioanal. Nucl. Chem.,* 288 (2011) 389-394.

3. Chromatographic separation of carrier free 90Y from 90Sr using a diglycolamide based resin for possible pharmaceutical applications, S. Dutta, P.K. Mohapatra, D.R. Raut, V.K. Manchanda, *J. Chromatogr.,* 1218 (37) (2011) 6483-6488.

4. Role of Diluent on the Separation of 90Y and 90Sr by Solvent Extraction and Supported Liquid Membrane Using T2EHDGA as the Extractant, S. Dutta, P.K. Mohapatra, D.R.Raut and V.K. Manchanda. *Appl. Radiat. Isot.*, (In press).

5. Separation of 90Y and 90Sr by TODGA as the carrier extractant: Solvent extraction and supported liquid membrane studies, S. Dutta, P.K. Mohapatra, D.R. Raut and V.K. Manchanda. *Sep. Sci. Technol.*, (communicated).

Symposia:

1. Studies on diluent effect on extraction and facilitated transport of Y(III) from nitric acid medium using TODGA, S. Dutta, P.K. Mohapatra, D.R. Raut and V.K. Manchanda, *In proceedings of DAE-BRNS Symposium on Nuclear and Radiochemistry (NUCAR-2011), held at GITAM University, Visakhapatnam during February* 22-26, 2011, pp. 316-317.

2. Separation of carrier free 90Y using supported liquid membrane containing TODGA as the carrier, S. Dutta, P.K. Mohapatra, D.R. Raut and V.K. Manchanda, *In proceedings of*

3. Separation of 90Y from 90Sr using N,N,N',N'-tetra-2-ethylhexyl diglycolamide (T2EHDGA) as the Extractant, S. Dutta, P.K. Mohapatra, D.R. Raut, V.K. Manchanda, *In proceedings of DAE-BRNS Symposium on Emerging Trends in Separation Science and Technology (SESTEC-2010) held at IGCAR, Kalpakkam, India, during March 1 -4, 2010,* pp. 605-606.

4. Modifier optimization and separation of carrier free 90Y using N,N,N',N'-tetra-2- ethylhexyl diglycolamide (T2EHDGA), S. Dutta, P.K. Mohapatra, D.R. Raut, V.K. Manchanda, *In proceedings of DAE-BRNS Symposium on Emerging Trends in Separation Science and Technology (SESTEC-2010) held at IGCAR, Kalpakkam, India, during March* 1 -4, 2010, pp. 607-608.

5. Separation of 90Y from 90Sr Using a TODGA Sorbed Extraction Chromatography Resin Material, S. Dutta, P.K. Mohapatra and V.K. Manchanda, *In proceedings of 'Indian Analytical Science Congress'- IASC-2009 held at Lonvala, Maharashtra, during Nov.* 12- 13, 2009, pp 42.

6. Studies on Relative Transport Behavior of 90Y and 90Sr across Supported Liquid Membrane Containing T2EHDGA as the Carrier, S. Dutta, D.R. Raut, P.K. Mohapatra and V.K. Manchanda, *In proceedings of 2nd International Conference on 'Application of Radiotracers in Chemical, Environment and Biological Science' - ARCEB - 10 held at Saha Institute of Nuclear Physics, Kolkata, during Nov.* 7-13, 2010, pp 164.

Name	:	**Imran Ali Khan**
Enrolment No.	:	ENGG01200704002
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Strength Mismatch Effects on Weld Centre Cracks Under Mode-I Loading: Analytical and Numerical Investigation

Abstract

Welding is one of the most widely used fabrication process in the nuclear power plants. It has been observed that weld joint locations are generally critical in comparison to base metal and, thus, their fracture integrity must be assured. Conventional defect assessment procedures that are being used at present were essentially developed for cracks lying in a homogeneous material. In view of the variations in the tensile and fracture properties of base and weld material, the integrity assessment of strength mismatch welds is not straightforward. Extensive studies are required on weld joints as besides specimen geometry and loading conditions the strength mismatch ratio M (defined as ratio of yield strength of weld to yield strength of base material) and weld slenderness ratio ψ (defined as ratio of uncracked ligament to half weld thickness) are the additional variables affecting the fracture assessment procedures. The present investigation is an effort in that direction.

In this work, a new load bounding technique, Modified Upper Bound (MUB) theorem, was proposed. Rigorous mathematical basis of this load bounding technique and its equivalence with the classical Slip Line Field analysis (SLF) was presented. Various simplifications resulting from the use of this new load bounding technique over SLF method were demonstrated. Apart from analysing standard homogeneous fracture mechanics specimens, the proposed MUB method was used to analyse weld strength mismatch effects. Application of the MUB method to the practical problem of evaluation of the limit load, plastic η-factor (used for experimental evaluation of fracture toughness), and crack tip stress fields of fracture specimens having weld centre crack was demonstrated. Aspects related to state of stress at the base-weld interface were discussed in detail. Excellent agreement was observed between the proposed theoretical solutions and those obtained from detailed full-field finite element analysis.

In addition, the important concern of characterization of crack-tip stresses in incompressible elastic-perfectly plastic material under mode-I loading was dealt with. A novel 5-sector formulation was developed to describe crack tip stresses. A new

constraint-indexing parameter T_{CS-2} was proposed which along with hydrostatic stress ahead of crack tip is capable of representing the entire elastic plastic crack-tip stress fields over all angles around a crack tip. It was demonstrated that the proposed constraint parameters are adequate to represent the effects of specimen geometry, loading conditions as well as weld mismatch on crack tip stresses.

Finally, modifications were proposed in the conventional fracture toughness estimation procedure so that a realistic evaluation of fracture toughness of weldments can be carried out. It is expected that the detailed analytical and numerical studies performed in this work would provide a comprehensive understanding of the effects of weld strength mismatch on the plasticity and fracture aspects of weld joints.

Publications

1. An insight of the structure of stress fields for stationary crack in strength mismatch weld underplane strain mode-I loading- Part I: Pure Bending Specimen. I.A. Khan, V. Bhasin, J.Chattopadhyay, and A.K. Ghosh, *International Journal of Mechanical Sciences, 2012, (InPress).*

2. Characterisation of crack-tip stresses in elastic-perfectly plastic material under mode-I loading.I.A. Khan, V. Bhasin, J. Chattopadhyay and A.K. Ghosh, *International Journal of MechanicalSciences, 53, 2011, 207-216.*

3. On the equivalence of slip-line fields and work principles for rigid-plastic body in plane-strain.I.A. Khan, V. Bhasin, J. Chattopadhyay and A.K. Ghosh, *International Journal of Solids andStructures, 45, 2008, 6416-6435.*

4. A Modified Upper Bound Approach to limit analysis for plane strain deeply crackedspecimens. I.A. Khan and A.K. Ghosh, *International Journal of Solids and Structures, 44,2007, 3114-3135.*International Conferences: 04

5. Analytical evaluation of crack tip constraint for rigid plastic material using Work principles.I.A. Khan, V. Bhasin, J. Chattopadhyay, K.K. Vaze, and A.K. Ghosh, *21st Int. Conf. on Struct.Mech. in Reactor Tech. (SMiRT-21)*, New Delhi, November 6-11, 2011.

6. Two parameter characterisation of crack tip stress field in elastic-perfectly plastic material. I.A.Khan, V. Bhasin, J. Chattopadhyay, K.K. Vaze, and A.K. Ghosh, *21st Int. Conf. on Struct.Mech. in Reactor Tech. (SMiRT-21)*, New Delhi, November 6-11, 2011.

7. Fracture mechanics evaluation of similar and dissimilar welded fracture specimens in planestrain.I.A. Khan, V. Bhasin, J. Chattopadhyay, K.K. Vaze, A.K. Ghosh, and H.S. Kushwaha,*20th Int. Conf. on Struct. Mech. in Reactor Tech. (SMiRT-20)*, Espoo, Finland, August 9-14,2009.

8. Structural Integrity assessment of welds, I.A. Khan, V. Bhasin, J. Chattopadhyay and A.K.Ghosh, *Inter-quadrennial Conf. of the Int. Congress on Fracture, IQCICF-08,* IISc.,Bangalore, August 4-7, 2008.

Name	:	**Swati Ghosh**
Enrolment No.	:	ENGG01200904016
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Effectof surface Working Operations on Electrochemical Corrosion and Susceptibility to Stress Corrosion Cracking of 304L Stainless Steel

Abstract

Mechanistic understanding of the effect of surface working operations on the electrochemical, oxidation and stress corrosion cracking (SCC) behavior of 304L austenitic stainless steel at ambient and at high temperature (300 °C) has been developed in this study. The effect of residual stresses induced by various fabrication techniques like tube straightening, roll-expansion, machining and grinding operations on the SCC susceptibility of stainless steel has also been studied. Solution annealed stainless steel grade 304 L was subjected to three different conditions: a) machining, b) grinding and c) cold rolling. This is followed by detailed microstructural characterization using optical, scanning electron microscopy (SEM), atomic force microscopy (AFM) and confirmation of phase transformations by X-ray diffraction (XRD) and electron back scattered diffraction (EBSD) studies. SCC susceptibility was evaluated by exposing constant strain samples made from each of the three conditions in 1 M HCl solution at room temperature (26 °C). Effect of residual stresses on susceptibility to chloride induced SCC was studied as per ASTM G36. The electrochemical nature of the as worked surfaces was studied at ambient temperature by potentiodynamic polarization, electrochemical impedance spectroscopy (EIS) and scanning electrochemical microscopy (SECM). Oxidation behavior of the material subjected to different surface finishing operations was followed in-situ by contact electric resistance (CER) and EIS measurements using controlled distance electrochemistry (CDE) technique in deaerated high purity water (specific conductivity < 0.1 μScm-1) at 300°C and 10 MPa in an autoclave connected to a recirculation loop system. The resultant oxide layer produced after 360 h exposure was characterized for a) elemental analyses by glow discharge optical emission spectroscopy (GDOES) and b) morphology by SEM. Results show that surface working operations drastically increased the SCC susceptibility of 304L stainless steel. This was shown to occur due to the formation of a work hardened surface layer constituted of sub micron grain size, martensite phase and high density of slip bands. The high temperature and high pressure studies on the oxidation behavior of surfaces in machined, ground and solution annealed conditions showed that surface working brings about major changes

in the oxidation behavior of stainless steel surfaces and the nature of the oxide film formed. Electrochemical polarization studies of the surfaces under different conditions revealed a) early onset of transpassivity and b) higher passive current densities as a result of surface working of 304L stainless steel. The oxide formed in case of machined and ground conditions is shown to have higher specific resistivity and richer in chromium content. The thickness of the oxide film formed after similar exposure period is the highest for solution annealed condition followed by machined and ground conditions. Presence of an additional ionic transport process during oxidation has also been identified for ground condition at the metal/oxide interface.

Publications

1. Swati Ghosh, M. Kiran Kumar, Vivekanand Kain, "Effect of surface working on high temperature oxidation behavior of 304L austenitic stainless steel by in-situ electrochemistry and oxide depth profiling, accepted by Corrosion Science, (2012).

2. Swati Ghosh, A. Khandelwal, Vivekanand Kain, A. Kumar, I. Samajdar, "Effect of surface working on the micro-electrochemical behavior of 304L stainless steel", accepted by Materials Characterization, (2012).

3. Swati Ghosh, Vishav Preet Singh Rana, Vivekanand Kain, Vivek Mittal and S. K. Baveja "Role of residual stresses induced by industrial fabrication on stress corrosion cracking susceptibility of austenitic stainless steel" Materials and Design, 32 (2011) pp. 3823–3831

4. Swati Ghosh, Vivekanand Kain, "Effect of surface machining and cold working on the ambient temperature chloride stress corrosion cracking susceptibility of AISI 304L stainless steel", Materials Science and Engineering: A, 527 (2010) pp. 679-693.

5. Swati Ghosh, Vivekanand Kain, "Microstructural changes in AISI 304L stainless steel due to surface machining : effect on its susceptibility to chloride stress corrosion cracking", Journal of Nuclear Materials, 403(2010) pp 62-67. Conference Proceedings

6. Swati Ghosh, M Kiran Kumar, Vivekanand Kain, "The effect of surface working on the hightemperature oxidation behavior of 304L stainless steel", proceedings of CORCON 2011 , No.22.

7. M. Kiran Kumar, Swati Ghosh and Vivekanand Kain, "Controlled Distance Electrochemistry (CDE) for High Temperature Oxidation Studies in Low Conducting Electrolytes − Application to Stainless Steels and Zirconium Alloys", submitted to ISEAC 2011.

8. Swati Ghosh and Vivekanand Kain, 'Understanding the effect of surface machining of 304L stainless steel by in-situ electrochemical study at high temperature and pressure', CD proceedings of 'Electrochem-2010: Electrochemistry and Sustainability', held from 13-17 September at Wolverampton, 2010.

9. Swati Ghosh, Vivekanand Kain, Vivek Mittal and S. K. Baveja, "Effect of residual stress and strain generated during manufacturing process on the stress corrosion cracking susceptibility of austenitic stainless steel" proceedings of the conference Corrosion, NACE International, Houston, 14-18, March, 2010. 128

10. Swati Ghosh and Vivekanand Kain, "Effect of microstructural changes induced by different stages of fabrication on chloride stress corrosion cracking susceptibility of AISI 304L at ambient temperature", proceedings of Environmentally assisted cracking, Vadodara, 6-9 th December, 2009.

Name	:	**Jhilam Sadhukhan**
Enrolment No.	:	PHYS04200804003
Constituent Institute	:	Variable Energy Cyclotron Centre, Kolkatta
Title	:	The stastical and Dynamical Models of Nuclear Fission

Publications

(A) Relevant to the present Thesis In refereed journals

1. Spin dependence of the modified Kramers width of nuclear fission, *Jhilam Sadhukhan* and Santanu Pal, Phys. Rev. C 78, 011603(R) (2008); Phys. Rev. C 79, 019901(E) (2009).

2. Critical comparison of Kramers' fission width with the stationary width from Langevin equation, *Jhilam Sadhukhan* and Santanu Pal, Phys. Rev. C 79, 064606 (2009).

3. Role of shape dependence of dissipation on nuclear fission, *Jhilam Sadhukhan* and Santanu Pal, Phys. Rev. C 81, 031602(R) (2010).

4. Fission as diffusion of a Brownian particle with variable inertia, *Jhilam Sadhukhan* and Santanu Pal, Phys. Rev. C 82, 021601(R) (2010).

5. Role of saddle-to-scission dynamics in fission fragment mass distribution, *Jhilam Sadhukhan* and Santanu Pal, Phys. Rev. C 84, 044610 (2011).

In conferences

1. A statistical model calculation for fission fragment mass distribution, *Jhilam Sadhukhan* and Santanu Pal, Proc. DAE-BRNS Symp. on Nucl. Phys. 52, 337 (2007).

2. A statistical model calculation of pre-scission neutron multiplicity with spin dependent fission width, *Jhilam Sadhukhan* and Santanu Pal, Proc. DAE-BRNS Symp. on Nucl. Phys. 53, 383 (2008).

3. A critical comparison of Kramers' fission width with the stationary width from Langevin equation, *Jhilam Sadhukhan* and Santanu Pal, Proc. DAE-BRNS Symp. on Nucl. Phys. 53, 453 (2008).

4. Fission as diffusion of a Brownian particle with variable inertia, *Jhilam Sadhukhan* and Santanu Pal, Proc. DAE-BRNS Int. Symp. on Nucl. Phys. 54, 362 (2009).

5. Role of shape-dependence of dissipation on nuclear fission, *Jhilam Sadhukhan* and Santanu Pal, Proc. DAE-BRNS Int. Symp. on Nucl. Phys. 54, 364 (2009).

6. Role of saddle-to-scission dynamics in fission fragment mass distribution, *Jhilam Sadhukhan* and Santanu Pal, Proc. DAE-BRNS Symp. on Nucl. Phys. 55, 270 (2010).

7. Fission width for different mass fragmentation from Langevin equations, *Jhilam Sadhukhan* and Santanu Pal, Proc. DAE-BRNS Symp. on Nucl. Phys. 55, 322 (2010).

8. Statistical and dynamical models of fission fragment mass distribution, *Jhilam Sadhukhan* and Santanu Pal, Proc. DAE-BRNS Symp. on Nucl. Phys. 56, 458 (2011).

9. Fission fragment mass distribution from combined dynamical and statistical model of fission including evaporation, *Jhilam Sadhukhan* and Santanu Pal, Proc. DAE-BRNS Symp. on Nucl. Phys. 56, 534 (2011).

(B) Other publications (in refereed journals)

1. The role of neck degree of freedom in nuclear fission, Santanu Pal, Gargi Chaudhuri, *Jhilam Sadhukhan*, Nucl. Phys. A 808, 1 (2008).

2. Evaporation residue excitation function from complete fusion of 19F with 184W, S. Nath, P. V. Madhusudhana Rao, Santanu Pal, J. Gehlot, E. Prasad, Gayatri Mohanto, Sunil Kalkal, *Jhilam Sadhukhan*, P. D. Shidling, K. S. Golda, A. Jhingan, N. Madhavan, S. Muralithar and A. K. Sinha, Phys. Rev. C 81, 064601 (2010).

3. Evidence of quasifission in the 16O+238U reaction at sub-barrier energies, K. Banerjee, T. K. Ghosh, S. Bhattacharya, C. Bhattacharya, S. Kundu, T. K. Rana, G. Mukherjee, J. K. Meena, *Jhilam Sadhukhan*, S. Pal, P. Bhattacharya, K. S. Golda, P. Sugathan, and R. P. Singh, Phys. Rev. C 83, 024605 (2011).

4. Angular momentum distribution for the formation of evaporation residues in fusion of 19F with 184W near the Coulomb barrier, S. Nath, J. Gehlot, E. Prasad, *Jhilam Sadhukhan*, P. D. Shidling, N. Madhavan, S. Muralithar, K. S. Golda, A. Jhingan, T. Varughese, P. V. Madhusudhana Rao, A. K. Sinha and Santanu Pal, Nucl. Phys. A 850, 22 (2011).

5. Evaporation residue excitation function measurement for 16O+194Pt reaction, E. Prasad, . K. M. Varier, N. Madhavan, S. Nath, J. Gehlot, Sunil Kalkal, *Jhilam Sadhukhan*, G. Mohanto, P. Sugathan, A. Jhingan, B. R. S. Babu, T. Varughese, K. S. Golda, B. P. Ajith Kumar, B. Satheesh, Santanu Pal, R. Singh, A. K. Sinha, and S. Kailas, Phys. Rev. C 84, 064606 (2011).

Name : **Soumen Samanta**
Enrolment No. : PHYS01200904004
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Charge Transport Studies in Organic Semiconductor Films

Abstract

This research work deals with growth and characterization of iron phthalocyanine (FePe) and cobalt phthalocyanine (CoPc) thin films on different substrates viz. glass, (0001) sapphire, (001) $LaAlO_3$, (001) $SrTio_3$ and 36.8º $SrTiO_3$ bi-crystal using molecular beam epitaxy (MBE) aiming to improve charge carrier mobility and study their charge properties as a function of temperature and bias. It has been shown that in the inert surface e.g.glass the molecules orient randomly. If the molecule substrate interaction is strong e.g. (0001) sapphire crystals, Pc molecules pack in the face-on configuration. In the cases resulting films are polycrystalline in nature. However, if the substrate has controlled surface roughness e.g.natural twinned boundaries present in the (001) $LaAlO_3$ single crystals, then molecules pack in the edge-on stacking along the twin boundaries. Similarly, phthalocyanine molecule order along single bi-crystal boundary when deposited on 36.8º cut (001) $SrTiO_3$ bi-crystal substrates.

The degree of ordering of phthalocyanine molecules in different substrates affects its charge transport properties. We have demonstrated that by choosing appropriate substrate, the mobility can be enhanced from <0.5 cm2V-1s-1(obtain for amorphous CoPc films on glass) to ~150 cm_2V-1s-1 (for highly ordered CoPc films grown along the 38.6º grain boundary of bicrystal $SrTiO_3$) which is the highest reported value till date. We have studied the charge transport properties of all the low and high mobility phthalocyanine films grown on different substrates. We have shown that the chemisorptions of ambient oxygen by CoPc films on glass lead to deep-traps, which results in hysteretic J-V characteristics described by deep trap limited space charge limited conduction (SCLC). The low temperature transport properties in this case are dominated by poole Frankel mechanism. On the other hand shallow traps in CoPc films, deposited on single crystalline sapphire, results in non-hysteretic J-V characteristics that can be described by trap-free SCLC in the entire investigated temperature range (300-75 K). High mobility of CoPc films, deposited along twin boundaries of (001) $LaAlO_3$ and along the 36.8º grain boundary of bicrystal SrTiO3 help us to investigate the charge transport properties of these films down to 20K. A new bias-temperature phase diagram has been proposed based on the charge

transport date. It has been shown that the charge transport is governed by bulk transport in high temperature region (>100K), which undergoes a bias dependent change from ohmic to trap-free space charge limited conduction. Whereas at low temperatures (<100K), the charge transport is dominated by contact limited processes, which changes from Schottky to multistep tunneling as a function of applied bias. We have also demonstrated that the conductivity of the films deposited along the boundry of SrTiO3 bi-crystal is in critical region.

We have alos demonstrated the applicability of ordered CoPc films for the ppb level Cl_2 sensing. The CoPc chemiresistive sensor, exhibit faster response times (18 s), higher base-line stabilities (<5% drift) and enhanced sensitivity (80%) for 5 ppb Cl_2.

Publications

Book Chapter

1. Organic semiconductor films for chemiresistor gas sensor; A. Singh, A. K. Debnath, D. K. Aswal, A. Joshi, S. Samanta, V. Saxena, S. K. Gupta, J. V. Yakhmi, in *Molecular and Organic Electronics*, D.K. Aswal and J.V. Yakhmi (eds), Nova Science Publisher, New York, 2010. ISBN: 978-1-66-594-2.

Refereed Journal

1. nfluence of adsorbed oxygen on charge transport and chlorine gas sensing characteristics of cobalt phthalocyanine thin films; S. Samanta, A. Kumar, A. Singh, A. K. Debnath, D. K. Aswal, S. K. Gupta, *Chem. Papers* (2012, at press).

2. Improved charge conduction in cobalt-phthalocyanine thin films grown along 36.8° boundary of SrTiO3 bicrystals; S. Samanta, A. Singh, A. Kumar, A. K. Debnath, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, *Appl. Phys. Lett.* 98 143301 (2011).

3. Bias and temperature dependent charge transport in high mobility cobaltphthalocyanine thin films; S. Samanta, D. K. Aswal, A. Singh, A.K. Debnath, M. S. Kumar, Y. Hayakawa, S. Gupta, J.V. Yakhmi, *Appl. Phys. Lett.* 96 013305 (2010).

4. Role of structural disorder in charge transport properties of cobalt-phthalocyanine thin films grown by molecular beam epitaxy; A. Singh, S. Samanta, A. Kumar, A. K. Debnath, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, Y. Hayakawa S. K. Deshpande, *Org Electron.* 11 1835 (2010).

5. Temperature dependent current-voltage characteristics of iron-phthalocyainthine films; S. Samanta, A. K. Debnath, A. Singh, D. K. Aswal, S. K. Gupta J. V. Yakhmi, *J. Nanosci. Nanotechnol.* 9 5262 (2009).

6. Parts-per-billion level chlorine sensors with fast kinetics using ultrathin cobalt phthalocyanine films; A. K. Debnath, S. Samanta, A. Singh, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, *Chem. Phys. Lett.* 480 185 (2009).

7. Oxygen induced hysteritc current-voltage characteristics of iron-phthallocyanine thin films; S. Samanta, A. Singh, A. K. Debnath, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, S. Singh, S. Basu, S. K. Deshpande, *J Appl. Phys* 104 073717 (2008).

8. Growth of iron phthalocyanine nanoweb and nanobrush using molecular beam epitaxy; A. K. Debnath S. Samanta, A. Singh, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, S. K. Deshpande, A. K. Poswal C. Sürgers, *Physica E* 41 154 (2008).

Conference Proceedings

1. Charge transport of ultrathin CoPc films on (001) LaAlO3 substrate; S. Samanta, A. Kumar, A. Singh, A. K. Debnath, D. K. Aswal, S. K. Gupta, *AIP Conference Proceedings of TFST, 2011. (to be published)*

2. Ordering induced enhancement of charge carrier mobility in CoPc thin films; S. Samanta, A. Singh, A. Kumar, A. K. Debnath, D. K. Aswal, S. K. Gupta, J. V.Yakhmi, *AIP Conference Proceedings 55th DAE solid state physics symposium* 1349 1043 (2010).

3. Implication of structural disorder in the charge transport properties of cobaltphthalocyanine thin films; A. K. Debnath, A. Kumar, S. Samanta, A. Singh, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, *AIP Conference Proceedings of 55th DAE solid state physics symposium* 1349 1047-1048 (2010).

4. Charge transport characteristics of Cobalt phthalocyanine thin films grown by molecular beam epitaxy; S. K. Gupta, A. Singh, S. Samanta, A. Kumar, A. K. Debnath, D. K. Aswal, *AIP Conference Proceedings of Physics of emerging functional materials* 1313 60 (2010).

5. stimation of ppb level chlorine concentration using Elovich equation; A. K. Debnath, A. Singh, S. Samanta, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, *Proc. 54th DAE Soild State Physics Symposium,* M. S. University, Vadodara, (2009).

6. Substrate dependent growth and electrical charge transport property of cobalt phthalocyanine thin films; S. Samanta, A. Singh, A. K. Debnath, D. K. Aswal, S. K. Gupta, J.V.Yakhmi, *Proc. International Symosium on Nanostructured Materials: Structure, properties and applications*, Jalandhar, (2009).

8. Selective chlorine gas sensors using cobalt phthalocyanine thin films; A. K. Debnath, A. Singh, S. Samanta, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, *Proc. 53rd DAE Soild State Physics Symposium*, Mumbai, (2008).

7. Molecular Beam Epitaxy Growth of Iron Phthalocyanine Nanostructures; A.K. Debnath, S. Samanta, A. Singh, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, *AIP conference proceedings of ICTOPON* 1147 347 (2009).

9. Temperature dependent current-voltage characteristics of iron-phthalocyainthine films; S. Samanta, A. K. Debnath, A. Singh, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, *Proc. of ICONSAT-08*, Chennai, (2008).

10. Hysteretic current-voltage characteristics of iron-phthalocyainthine films; S. Samanta, A. K. Debnath, A. Singh, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, *Proc. 52rd DAE Soild State Physics Symposium*, Mysore, (2007).

11. Surface morphology and gas sensing characteristics of the iron-phthalocyainthine thim films; A. K. Debnath, S. Samanta, A. Joshi, A. Singh, D. K. Aswal, S. K. Gupta, J. V. Yakhmi, *Proc. 52rd DAE Soild State Physics Symposium*, Mysore, (2007).

Name	:	**Asavari Santosh Dhavale**
Enrolment No.	:	PHYS01200704012
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Study of RF Structures for Linear Accelerators

Abstract

Particle accelerator technology has tremendous usage in the field of industry as well as basic sciences. Considering the potential of this field, Accelerator and Pulse Power Division (APPD) has taken up several accelerator development projects. Of this, development of linear accelerators for the industrial purpose like irradiation of cables, spices, medical equipment etc. is the main divisional activity. Another project of national interest is the development of Accelerator Driven Subcritical System (ADSS) that will be mainly utilized for the transmutation of nuclear waste. It involves development of RF accelerator system to accelerate proton beam from 50 keV to 1 GeV. The proton beam generated by ion source will be accelerated upto 100 MeV by various stages of normal conducting accelerating structures viz., RFQ, CCDTL, CCL. The last module that will accelerate proton beam from 100 MeV to 1 GeV (β>0.42) will be superconducting coupled cavity structure made up of elliptical cavities. Generally for low proton energy (β<0.3), Quarter Wave Resonator, Spoke type cavities are more popular whereas at higher energies (β>0.6) Elliptical cavities are more suitable. As superconducting structures can provide larger field gradient they are compact as compared to normal conducting accelerator structure and hence are preferred. All over the world lot of research and development work is going on in this field.

In any RF accelerator system, RF cavity and the input power coupler are the most vital subsystems. The amount of power coupled to the structure depends on the coupling between cavity and the coupler. Any mismatch at the coupler results in the improper field gradient as well as the reflection of RF power at the source side. This in turn can damage to the other components present in the transmission line like directional coupler, circulator, ceramic windows etc. Thus a careful study of cavity and the coupler parameters and optimization of the coupling factor between cavity resonator and the input coupler is essential. The thesis will cover the theoretical and experimental study of the RF cavities, Input Coupler for RF Linear Accelerators. The theoretical study involves the computation of cavity parameters, coupling factor using standard codes. It involves the comparative study of different type of couplers, study of dependence of coupling factor on the various cavity and coupler parameters and also the physical parameters like beam loading. The experimental work will cover the RF characterization of the Cavity, Coupler parameters. Also the study of multipacting phenomena in the coupler and the study of materials will be carried out.

Publications

Journal Papers

1. A.S.Dhavale, P.Dhakal, A.A. Polyanskii, G. Ciovati, "Flux pinning characteristics in cylindrical niobium samples used for superconducting radio frequency cavity fabrication", Supercond. Sci and Technology, 25(2012), 065014, doi:10.1088/0953.2048/25/6/065014

2. A.S.Dhavale and K.C.Mittal, "Multipacting analysis of power coupler for SC cavity", *Nuc. Instr. & Methods in Physics A*, 677 (2012), 25-30

3. A.S.Dhavale and K.C.Mittal, "RF chracterization of elliptical prototype copper cavity and the power coupler", *Journal of Instrumentation, JINST*, 4 T 09002, 2009.

4. A.S.Dhavale and K.C.Mittal "Design of Input Coupler for the superconducting cavity", *Nuclear Instruments and Methods in Physics Research A*, Volume 604, Issue 3, 11 June 2009, doi: 10.1016/j.nima.2009.03.176 36

5. A.S.Dhavale and K.C.Mittal, "Evaluation of External Q using Kroll-Yu Method with Microwave Studio", *Journal of Instrumentation*, *JINST*, 3 T06001, 2008.

International Conference/ Symposium

1. A.S.Dhavale and K.C.Mittal, "Study of Mutipacting in coaxial coupler", IPAC10, Kyoto, Japan, 2010

2. A.S.Dhavale, G.Ciovati and G.R.Myneni, "Effect of Electropolishing and Low Temperature Baking on the Superconducting Properties of Large-Grain Niobium", Symposium on Superconducting Sci. and Technology of Ingot Niobium (SSTIN10), Sep. 22-24, 2010, TJNAF, Newport News, VA

National Conference

1. K.C.Mittal, A.S.Dhavale et.al., "SCRF Program at BARC", InPAC 2009, RRCAT, Indore

Name   :   **Sutapa Saha**
Enrolment No.   :   LIFE05200704001
Constituent Institute   :   Saha Institute of Nuclear Physics, Kolkata
Title   :   roteomic Study in a Haematological Malignancy: B-Cell Acute
                                  Lymphoblastic Leukemia

Publications

1. Saha, S., Banerjee, S., Banerjee, D., Chandra, S., Chakrabarti, A. Differentially regulated CD19+ B-lymphocyte proteome in B-cell Acute Lymphoblastic Leukemia: Biological insights. (*Communicated*)

2. Saha, S., Halder, S., Bhattacharya, D., Banerjee, D., Chakrabarti, A. Altered plasma levels of proteolysis-modulating, carrier and acute phase proteins in B-cell Acute Lymphoblastic Leukemia. (*Communicated*)

3. Saha, S., Ramanathan, R., Basu, A., Banerjee, D., and Chakrabarti, A. (2011) Elevated levels of redox regulators, membrane bound globin chains and cytoskeletal protein fragments in hereditary spherocytosis erythrocyte proteome. *Eur J Haematol*. (In Press)

4. Chakrabarti, A., Bhattacharya, D., Basu, A., Basu, S., Saha, S., and Halder, S. (2011) Differential expression of red cell proteins in hemoglobinopathy. *Proteomics Clin Appl* 5, 98- 108.

5. Bhattacharya, D., Saha, S., Basu, S., Chakravarty, S., Chakravarty, A., Banerjee, D., and Chakrabarti, A. (2010) Differential regulation of redox proteins and chaperones in HbEbetathalassemia erythrocyte proteome. *Proteomics Clin Appl* 4, 480-488.

6. Chakrabarti, A., Datta, P., Bhattacharya, D., Basu, S., and Saha, S. (2008) Oxidative crosslinking, spectrin and membrane interactions of hemoglobin mixtures in HbEbetathalassemia. *Hematology* 13, 361-368.

7. Banerjee, D., Saha, S., Basu, S., and Chakrabarti, A. (2008) Porous red cell ultrastructure and loss of membrane asymmetry in a novel case of hemolytic anemia. *Eur J Haematol* 81, 399-402.

List of seminars and workshops attended

1. Oral Presentation at the 47th Annual Conference of the Indian Society of Haematology & ransfusion Medicine, Guwahati Medical College, Guwahati,

2. November 24-26, 2006, on Proteomics in the study of hematological malignancies.

3. Workshop on iTRAQ Technology for Quantitative Proteomics, Centre for Cell and Molecular Biology, Hyderabad, August 27-29, 2007.

4. Oral Presentation at CME 2007 Scientific Meet on Haemato-Oncology, Netaji Subhash Chandra Bose Cancer Research Institute, Taj Bengal, Kolkata, September 8-9, 2007, on Proteomics in the study of hematological malignancies.

5. Poster Presentation at the International Symposium on Complex Diseases: Approaches to Gene Identification and Therapeutic Management, Saha Institute of Nuclear Physics, Kolkata, September 25-26, 2008, on Clinical Proteomics in Blood Disorders.

6. Presentation at the 11th ISMAS Triennial International Conference on Mass Spectrometry, 11th ISMAS-TRICON-2009, Ramoji Film City, Hyderabad, November 24-28, 2009, on "Salting out" the hidden plasma proteome.

7. Presentation at the National seminar on Proteomics: Advances, Applications and Challenges (PRAAC), Institute of Bioinformatics and Applied Biotechnology, Bangalore, February 19- 20, 2010, on Salting out the hidden plasma proteins implicated in B-ALL.

8. Poster Presentation and Oral Presentation at the 5th AOHUPO Congress, 14th ADNAT Convention & 1st PSI Conference of New Perspectives in Proteome Research, February 21-25, 2010, Centre for Cellular & Molecular Biology, Hyderabad, on Identification of disease regulated blood plasma proteins in B-ALL & Proteomics of CD19+ B cells implicated in acute ymphoblastic leukemia respectively.

Name	:	**Mohd. Nazir Khan**
Enrolment No.	:	LIFE01200704004
Constituent Institute	:	Saha Institute of Nuclear Physics, Kolkata
Title	:	Proteomic Study in a Haematological Malignancy: B-Cell Acute Lymphoblastic Leukemia

Abstract

Lionizing radiation is playing a key role in various aspects of human of life, and there is a great need to understand the mechanisms of radiation injury, which will help in harnessing the full potential of beneficial effects of Radiation to mankind, Agents that modify the effects of radiation are called radiomodifiers. These can be either radioprotectors (protest against radiation injury) or radiopotentiators (intensity the effect of radiation injury). Several approaches were used to modify the radiation effects; we have used a novel approach of cellular redox alteration for modification of radiation injury. We hypothesize that alteration in cellular redox can elicit oxidative stress which depending on magnitude of redox perturbation either stimulate prosurvival or proapaptotic pathways leading to radioprotentiation. In the present thesis, 1, 4 naphthoquinone (NQ) the parent molecule of many clinically approved drugs and unconjugated bilirubin (UCB) an endogenous degradation product of heme, have been evaluated for their radiomodifying activity.

Presence of NQ radiation exposure to lymphocytes inhibited radiation induced apoptosis. Being prooxidant in nature. When NQ was added to lymphocytes it perturbed the redox balance and activated redox sensitive transcription factor Nrf2 and increase the expression of cytoprotective gene hemeoxygenase – 1, which is responsible of observed radioprotection. NQ increased ERK phosphorylationw which is upstream to Nrf2 and this ERK activation was through increased intracellular calcium levels. Further, administration of NQ to mice offered protection against whole body irradiation induced apoptosis and mortality. Dose modification factor of NQ was found of NQ was found to be 1.18.

Treatment of lymphocytes with UCB at clinically relevant concentration induced apoptosis and further augmented the radiation induced apoptosis via induction of oxidative stress. The administration of UCB induced splenic atrophy, bone marrow aplasia and leucopenia and further potentiated the radiation effects. Further, UCB administration prior to radiation exposure deteriorated the host immune response and increased susceptibility to infection, sepsis and mortality in mice. In conclusions our results showed that mild oxidative stressor can be used as potential radioprotector where as serve oxidative stressor behave as cytotoxic agent and potential the effect of radiation.

Publications

In International Peer Reviewed Journal

1. Nazir M Khan, Sandur SK, Checker R, Sharma D, Poduval TB, Sainis KB. Prooxidants ameliorate radiation-induced apoptosis through activation of the calcium-ERK1/2-Nrf2 pathway. Free Radic Biol Med. 2011 Jul 1; 51(1):115-28. Epub 2011 Apr 8. PubMed PMID: 21530647.

2. Nazir M Khan, Poduval T.B. Immunomodulatory and Immunotoxic effects of bilirubin: Molecular mechanism. J. leuk. Biol. 2011 Nov; 90(5):997-1015. Epub 2011 Aug 1.PMID: 21807743.

3. Nazir M. Khan, Poduval T. B. Bilirubin augments radiation injury and leads to increased infection and mortality in mice: Molecular mechanisms. Free Radic Biol Med. (Accepted), 2012

4. Premachandran S, Nazir M. Khan, Thakur VS, Shukla J, Poduval T. B. Differential immunotoxic effects of ethanol on murine EL-4 lymphoma and normal lymphocytes is mediated through

5. increased ROS production and activation of p38MAPK. Immunopharmacology and Immunotoxicology, 2012 Aug; 34(4):616-26.

6. Wilankar C, Nazir M. Khan, Checker R., Sharma D., Patwardhan R.S., Gota V., Sandur S.K., Devasagayam T. P. A. γ-Tocotrienol Induces Apoptosis in Human T\ Cell Lymphoma through Activation of Both Intrinsic and Extrinsic Pathways:\ Curr Pharm Des, 2011, 17 (21) : 2176-89. PMID: 21774779.

7. Shukla J, Nazir M. Khan, Thakur VS, Poduval TB. L-Arginine Mitigates Radiation-Induced Early Changes in Cardiac Dysfunction: The Role of Inflammatory Pathways. Radiat Res. 2011 Aug; 176(2):158-69. Epub 2011 Jun 10. PMID: 2166339.

8. Checker R, Sharma D, Sandur SK, Nazir M. Khan, Patwardhan RS, Kohli V, Sainis KB. Vitamin K3 suppressed inflammatory and immune responses in a redox-dependent manner. Free Radic Res. 2011 Aug; 45(8):975-85. Epub 2011 Jun 9. PMID: 21651451.

9. Wilankar C, Sharma D, Checker R, Nazir M. Khan, Patwardhan R, Patil A, Sandur SK, Devasagayam TP. Role of immunoregulatory transcription factors in differential immunomodulatory effects of tocotrienols. Free Radic Biol Med. 2011 Jul1;51(1):129-43. Epub 2011 Apr 8. PubMed PMID: 21536125.

(C) In National Journal

1. Mohd Nazir Khan, Santosh Kumar Sandur, Rahul Checker, Deepak Sharma, T. B. Poduval and K.B. Sainis. Radioprotective Effects of Pro-oxidants. Advanced
Biotech, Journal of Biotechnology (ISSN:0973-0109) 2010, Nov; 10(05): 100 237

(D) In Conference/Symposia

1. Nazir M. Khan, Santosh Kumar Sandur, Rahul Checker, Deepak Sharma, and T. B. Poduval. 1,4 Naphthoquinone protect radiation induced death and DNA damage in lymphocyte by enhancement in DNA repair. International Conference on Emerging Frontiers and Challenges in Radiation Biology. Bikaner, India, January 24th – 25th, 2012.

2. Nazir M. Khan, H. N. Bhilwade, Rahul Checker, Deepak Sharma, Vikram Gota and Santosh K. Sandur. Withaferin-α offers radioprotection via activation of repair of radiation induced DNA strand breaks in lymphocytes. International Conference on —Emerging Trends in Free Radicals, Antioxidants and nutraceuticals on Health, Disease and Radiation Biology. Kolkata, India, January 2th -14th, 2012.

3. Chandan Wilankar C, Nazir M. Khan, Rahul Checker R., Deepak Sharma, Patwardhan R.S., Gota V., Sandur S.K., Devasagayam T. P. A. γ-Tocotrienol Induces Apoptosis in Human T Cell Lymphoma through Activation of Both Intrinsic and Extrinsic Pathways. International Conference on —Emerging Trends in Free Radicals, Antioxidants and nutraceuticals on Health, Disease and Radiation Biology. Kolkata, India, January 12th-14th, 2012.

4. Sudha Premachandran, Nazir M. Khan, Vikas S. Thakur, Jyoti Shukla, and T. B. Poduval. Differential immunotoxic effects of ethanol on murine EL-4 lymphoma and normal lymphocytes is mediated through increased ROS production and mactivation of p38MAPK. International Symposium on Innovation in Free Radical Research and Experimental Therapeutics, Coimbatore, India, December 7th-9th, 2011.

5. Goswami M, Deepak Sharma, Nazir M. Khan, Shweta Suryavanshi, Santosh Kumar Sandur, Narendra Jawali. Effects of Antioxidant on Streptomycin Mediated Clearance of Acute Bacterial Peritonitis in Swiss Albino Mice. International Conference on Recent Trends on Therapeutic Advancement of Free Radical Science, Chennai, India, January 9th-11th, 2011.

6. Mohd Nazir Khan, Santosh Kumar Sandur, Rahul Checker, Deepak Sharma, T. B. Poduval and K.B. Sainis. Radioprotective Effects of Pro-oxidants. International Conference on Radiation Biology: Nanotechnology, Imaging and Stem Cells in Radiation Oncology. Chennai, India, November 15th-17th, 2010.

7. Shweta Suryavanshi, Mohd Nazir Khan, Rahul Checker, Deepak Sharma, S. Santosh Kumar and K. B. Sainis Radioprotective Effects of Chlorophyllin on Hematopoietic System. International Conference on Advances in Free Radical Research: Natural Products, Antioxidants and Radioprotectors. Hyderabad, India, January 11th-13th, 2010.

8. Mohd Nazir Khan, Shweta Suryavanshi, Deepak Sharma, Rahul Checker, Sandur Santosh Kumar, T. B. Poduval. Investigation of the radioprotective efficacy of 1, 4-Naphthoquinone against gamma-radiation induced cellular damage in murine lymphocytes. International Conference on Advances in Free Radical Research: Natural Products, Antioxidants and Radioprotectors. January 11th-13th, 2010.

9. Mohd Nazir Khan, Rahul Checker, Deepak Sharma, Rashmi Raghu, S. Santosh Kumar and T. Balakrishna Poduval. Immunomodulation by NF-kappaB inhibitors 238 from natural sources. International Conference on Advances in Free Radical Research: Natural Products, Antioxidants and Radioprotectors. Lucknow, India, March 19th-21th, 2009.

10. Mohd Nazir Khan, Deepak Sharma, Rahul Checker, Rashmi Raghu, T. B. Poduval Radioprotective and Immunomodulatory Properties of Bilirubin. Life Sciences Symposium on Recent Advances in Immunomodulation in Stress and Cancer. Mumbai, India December 22th-24th, 2008.

(E) In News Letter

1. Nazir M. Khan, T. B. Poduval. Is antioxidant property, a better approach to find a radioprotector? Radiation Science Today, 2012, Issue 19, July, 4-6.

Oral Presentation:

1. Nazir M. Khan, Santosh Kumar Sandur, Rahul Checker, Deepak Sharma, and T. B. Poduval. 1,4 Naphthoquinone protect radiation induced death and DNA damage in lymphocyte by enhancement in DNA repair. International Conference on Emerging Frontiers and Challenges in Radiation Biology. Bikaner, India, January 24th-25th, 2012.

2. Mohd Nazir Khan, Santosh Kumar Sandur, Rahul Checker, Deepak Sharma, T. B. Poduval and K.B. Sainis. Radioprotective Effects of Pro-oxidants. International Conference on Radiation Biology: Nanotechnology, Imaging and Stem Cells inRadiation Oncology. Chennai, India, November 15th-17th, 2010.

Awards Received

1   My paper (J. leuk. Biol. 2011 Nov; 90(5):997-1015) was enlisted in the series publication by Global Medical Discovery, a Canadian based company serving alerts the scientific community to breaking journal articles considered to be of importance to the drug discovery Process.

2   Travel award from Indian Society of Radiation Biology for Oral presentation at International Conference on Emerging Frontiers and Challenges in Radiation Biology. Bikaner, India, January 24th – 25th, 2012.

3   Best Poster Award in International Conference on —Emerging Trends in Free Radicals, Antioxidants and Nutraceuticals on Health, Disease and Radiation Biology held in Kolkata, India, January 12th -14th, 2012.

Name   :   **Lalit Sehgal**

Enrolment No.   :   LIFE09200604002

Constituent Institute   :   Tata Memorial Centre, Mumbai

Title   :   Generation of Knockdown Mice That Lack 14-3-3ε and 14-3-
                                      3Υ using RNA Interference

Abstract

Lentiviral vectors are effective at delivering transgenes in a broad range of cell types. The present dissertation reports the development of HIV-1 based multiple lentiviral vectors that can be used to express shRNA's and cDNA's in cultured cells. These vectors were used to develop a new cost effective, rapid technique for the generation of transgenic mice, which has a high success rate. Briefly, spermatogonial stem cells are infected with lentiviral particles *in vivo*. . After sperm maturation, these fore-founder mice are mated with WT female mice to generate transgenic pups. This technology does not compromise the fertility of the off-spring, resulting in germline transmission of the transgene, using a limited number of animals. The procedure could be extended to other animals, especially non-human primates, resulting in a significant advancement in transgenic research and the use of other animal models to model human disease.

The results from this thesis demonstrated that mice injected with lentiviruses expressing shRNAs targeting 14-3-3γ were unable to sire pups when mated with WT female mice. A further analysis of the testes phenotype showed severe cell-cell adhesion defects, defects in spermatogenesis resulting in sterility. Cell-cell adhesion is required for the development of spermatocytes and spermatogenesis. To determine if 14-3-3γ loss leads to a defect in cell-cell adhesion, HCT116 cells lacking 14-3-3γ were used as a model system. Our results showed that 14-3-3γ is required for the transport of the desmosomal components to the cell border in both HCT116 cells and the mouse testis. We found that 14-3-3γ is required to load the desmosomal plaque protein plakoglobin (PG) onto the motor protein KIF5B, both in the presence or absence of calcium. Loss of 14-3-3γ disrupts loading of PG to KIF5B, and the recruitment of PG to the cell border is compromised. The absence of PG on cell border upon loss of 14-3-3γ fails to recruit other desmosomal proteins thereby halting initiation of desmosome formation. Similar results were obtained when KIF5B expression was inhibited in both HCT116 cells and mouse testis suggesting that 14-3-3γ is required for the KIF5B dependent transport of PG to the cell border.

The 14-3-3ε knockdown mice died nearly 6 months post birth. It has been reported earlier that mice heterozygous or homozygous null for 14-3-3ε have defects in brain development and neuronal migration. We observed that although the level of 14-3-3ε in brain is significantly reduced, cortical thinning was not observed. These mice showed pleotropic phenotypes including spleenomegaly and patchy hair loss. We observed lymphocytic infiltration in various organs (lung, liver and kidney) of the 14-3-3ε knockdown mice. The levels of CD3+ and CD4+ cells were significantly increased. Upon analysis we also found that the level of CD3+ CD4- CD8- cells is more in the knockdown mice, generally observed in patients with leukemia. These results therefore suggest that loss of 14-3-3ε may lead to neoplastic progression.

Publications

1. Lalit Sehgal, Rahul Thorat, Nileema Khapre, Amitabha Mukhopadhaya, Mugdha Sawant and Sorab N Dalal Lentiviral mediated transgenesis by in vivo manipulation of Spermatogonial stem cells. PLoS ONE 6(7): e21975.

2. Gosavi, P., S. T. Kundu, N. Khapare, Lalit Sehgal, M. S. Karkhanis, and S. N. Dalal. E-cadherin and plakoglobin recruit plakophilin3 to the cell border to initiate desmosome assembly. Cell. Mol. Life Sci. (2011) 68:1439–1454

3. Lalit Sehgal, Rahul Thorat, Nileema Khapre, Amitabha Mukhopadhaya, Mugdha Sawant and Sorab N Dalal. A protocol for generation of transgenic mice by manipulating spermatogonial stem cells in vivo. (Nature Protocol Exchange, 29 May, 2012).

4. Lalit Sehgal, Amitabha Mukhopadhaya, Anandi Rajan, Khyati Bhatt, Mugdha Sawant, Dipika Gupta, Rahul Thorat, Neelima Khapare, and Sorab N Dalal. Role of 14-3-3γ in cell-cell adhesion and mice sterility. (Manuscript under preparation).

5. Lalit Sehgal, Srikanth B., Khyati Bhatt, Sneha Sansare, Amitabha Mukhopadhayay, Rajiv D. Kalraiya , and Sorab N. Dalal. Generation of HIV-1 based bi-cistronic lentiviral vectors for stable gene expression and live cell imaging. (Accepted, Indian Journal of Experimental Biology).

Other publications.

1. Hunain Alam, Lalit Sehgal, Samrat T. Kundu, Sorab N. Dalal and Milind M.Vaidya Novel function of Keratin 5 and 14 in proliferation and differentiation of stratified epithelial cells. (Molecular biology of Cell, volume 22, November 1 2011, 4068-4078)

2. Hunain Alam, Amruta V. Bhate, Prakash Gangadaran, Sharda S. Sawant, Lalit Sehgal, Shimul Salot, Prerana P. Dange, Devendra A. Chaukar, Anil K D'cruz, Sadhna Kannan, Rajiv Gude, Shubhada Kane, Sorab N. Dalal and Milind M. Vaidya.Fascin overexpression promotes neoplastic progression in OSCC. (BMC Cancer. 2012 Jan 20;12(1):32).

3. Khapare N*, Lalit Sehgal*, S Kundu*, R Priya, Mugdha Sawant, P Gosavi, N Gupta, H Alam, M Karkhanis, N Naik, M M Vaidya, S N Dalal, Cytokeratin 8 stabilization is required for the transformation induced upon loss of plakophilin3 expression. (PLoS One. 2012; 7 (6):e38561. Epub 2012 Jun 6.) * These authors contributed equally.

Patents

1. Lalit sehgal, Rahul throat, Nileema Khapre and Sorab N Dalal; Lentiviral mediated transgenesis. (2010) Patent Governement of India (current status filed 2442/DEL/2010

2. Lalit sehgal, Rahul throat, Nileema Khapre and Sorab N Dalal; Lentiviral mediated transgenesis. (2011) Patent United States of America (current status filed 13004382 dated 11 January 2011)

Poster/oral Presentations.

1. Lalit Sehgal, Rahul Thorat, Nileema Khapre, Amitabha Mukhopadhaya and Sorab N Dalal Lentiviral mediated transgenesis by in-vivo manipulation of spermatogonial stem cells. Presented a poster at AACR *New Horizons in Cancer* 223 *Research: Biology to Prevention to Therapy* conference, Delhi , December 13-16, 2011.

2. Lalit Sehgal, Rahul Thorat, Nileema Khapre, Amitabha Mukhopadhaya and Sorab N Dalal Lentiviral mediated transgenesis using Sperm mediated gene transfer. Presented a Poster at 79th annual meeting of Society of biological chemistry Indian institute of Sciences, Bangalore 13th December 2010-15th December 2010.

3. Lalit Sehgal, Rahul Thorat, Nileema Khapre, Amitabha Mukhopadhaya, and Sorab N Dalal Lentiviral mediated transgenesis in vivo. Presented a poster at Mouse development, genetics and genomics meeting at Cold spring Harbor Laboratory, NY USA, 26th October 2010-30th October 2010.

4. Lalit Sehgal, Rahul Thorat, Nileema Khapre, Amitabha Mukhopadhaya, and Sorab N Dalal Generation of transgenic mice by Sperm mediated gene transfer.
    Presented a talk entitled "at 5th Graduate students meet at ACTREC 18 and 19th December 2009. Received third prize.

5. Lalit Sehgal, Rahul Thorat, Nileema Khapre, Amitabha Mukhopadhaya, and Sorab N Dalal Generation of knockdown mice by Sperm mediated gene transfer. Presented a poster at 33rd All India cell biology conference 2009 & international workshop on cell cycle regulation held at central university of Hyderabad, Hyderabad from 10th -13th December 2009.

6. Lalit Sehgal, Amitabha Mukhopadhaya, and Sorab N Dalal "Generation of stem cell lines and knockdown mice that lack 14-3-3ε and 14-3-3γ using RNA interference" Participated and presented a poster at international meeting on Model organism and stem cell biology at NCBS, Bangalore, Feb 23-25 2008.

Name	:	**Prasun Sharma Chowdhury**
Enrolment No.	:	PHYS04200604001
Constituent Institute	:	Variable Energy Cyclotron Centre, Kolkata
Title	:	Characterization of Microstructure of Nuclear Structural Materials by XRD

Abstract

The zirconium based alloys and stainless steels are very important core structural materials in nuclear reactors. These alloys show very good performance in the mechanical properties at elevated temperatures and sustain the structural integrity of the nuclear reactor under severe operating conditions. The important zirconium based alloys are the zircaloy-2, Zr-2.5Nb, Zr-1Nb, Zr-1Nb and Zirlo. On the other hand, the stainless steels like SS316L and D9 alloy are the important core structural materials for Fast Breeder Reactor (FBR). The pre-irradiation microstructure of these materials plays significant role in controlling their structural integrity during the operation of the reactors. Hence it is of great interest to study the microstructure of these alloys under deformed and irradiated conditions.

There are various well known techniques to study the microstructure of the polycrystalline materials like optical microscopy, X-ray diffraction technique, electron microscopy etc. Out of all these techniques, only the X-ray diffraction technique provides statistically averaged information about the microstructure of the materials over a large volume of the sample (-10^9 um^3), whereas the other techniques provide localized information about the microstructure of the materials.

In the present thesis, the microstructure of different zirconium and stainless steel based reactor core structural materials have been characterized using X-ray Diffraction Line Profile Analysis (XRDLPA). The studies have been performed under the deformed and irradiated conditions of the materials. The post-irradiation microstructural changes of the Zr-1Nb alloy have been characterized using XRDLPA. Positron Annihilation Spectroscopy (PAS) has been used to characterize the nature of the point defects created during irradiation of Zr-1Nb alloy and their role in controlling the irradiated microstructure. Anomalous variation was observed in the microstructural parameters at some specific dose of irradiated Zr-1 Nb alloy. This observation elucidates the fact that the irradiated microstructure is very much sensitive Zr-1 Nb alloy. This observation elucidated the fact that the irradiated microstructure is very much sensitive to dose and dose rate in the low dose regime.

Study of the deformed microstructure reported in this thesis can be classified into two different parts. In the first part, heavily deformed powders of different zirconium based alloys (Zircaloy-2, Zr-2.5Nb and Zirlo) have been obtained with the help of finely threaded jewelery files. The microstructures of these heavily deformed alloys have been characterized using the different model based techniques of XRDLPA. These different models of XRDLPA were found to be complementary to each other in characterizing the microstructure of the material. The studies show that, the presence of Nb enriched ⍺- phase in ⍺-Zr matrix in Zr-2.5Nb and Zirlo was responsible in controlling the domain growth, resulting in a smaller domain size compared to that of Zircaly-2.

In the second part, the in-situ microstructural evolution of heavily deformed D9 alloy powders has been studied during the early stages of annealing, both with time and temperature. In this study, the evolution of the lowest length scale dislocation substructure at the earliest stage of annealing has been studied for the first time using XRDLPA. The growth of these lowest length scale substructures during

the early stages of annealing have been modeled successfully from the light of the rearrangement and annihilation of dislocations.

Hence, the microstructural change of different nuclear structural materials during their irradiation, deformation and annealing, has been successfully studied using the different model based techniques of XRDLPA.

Publications

1. Studies of Microstructural Imperfections of powdered Zirconium Based alloys: P.S. Chowdhury, A.Sarkar, P. Mukherjee, N. Gayathri, M. Bhattacharya, P. Barat. Materials Characterization 61 (2010) 1061–1065.

2. In situ studies of evolution of microstructure with temperature in heavily deformed Ti-modified austenitic stainless steel by X-ray Diffraction technique: P.S. Chowdhury, N. Gayathri, P. Mukherjee, M. Bhattacharya, A. Chatterjee, A Dutta, P. Barat. Materials Science and Engineering A 528 (2011) 967–972.

3. Post irradiated microstructural characterization of Zr-1Nb alloy by X-ray diffraction technique and positron annihilation spectroscopy: P.S.Chowdhury, P.Mukherjee, N.Gayathri, M.Bhattacharya, A.Chatterjee, P.Barat, P.M.G Nambissan. Bulletin of Materials Science 34 (2011) 507-513.

Name	:	**Naresh Kumar Jena**
Enrolment No.	:	CHEM01200604003
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Computational Investigations on the Structure and Reactivity of Nanomaterials

Abstract

The thesis is organized into 7 chapters. In Chapter 1, a brief introduction to the broad spectrum of nanomaterials has been provided. This chapter also gives a preliminary account of the computational strategies employed for the study of nanomaterials. The scope of the present thesis is also outline in this introductory chapter. In chapter 2, the structure and electronic properties of carbon nanotubes (CNT) have discussed considering suitable model systems. The nanoscale curvature is shown to govern the electronic properties of CNT on the basis of correlation of several properties like dipole moment, polarizabilities etc. with the inherent curvature present in CNT. In the later part of this chapter, important structural and electronic properties of water under the confinement of CNT have been discussed in terms of model systems where two pertinent parameters namely confinement and curvature are shown to be of paramount importance. Chapter 3 delves with the structure, reactivity and possible applications of C_{60} fullerenes. This chapter is broadly divided into two parts where the first part deals with the structure, stability and non-linear optical properties of N-doped fullerenes (azafullerenes) with formula $C_{60-2n}N_{2n}$(n=1-12). In the second part of this chapter, functionalization of fullerenes with malonate is discussed in terms of their binding with uranyl cation and their possible role in nuclear waste management. The structure and electronic properties of pristine and doped gold nanoclusters Au_n (n=2-8) have been discussed in chapter 4. Variation of important electronic properties like ionization potential, electron affinity, HOMO-LUMO gap etc. with cluster size and variation of dopant atoms have been demonstrated. As a first step to understand the catalytic properties of gold clusters towards CO oxidation reaction, adsorption of CO molecule on these gold clusters towards CO oxidation reaction, adsorption of CO molecule on these gold clusters is investigated. Further, the substrate effect on CO adsorption is also studied by considering different carbon nanostructure surfaces. In chapter 5, investigations have been carried out to tune electronic properties of gold clusters for their role in efficient catalysis taking CO oxidation reaction as a case study. Doping of impurities like hydrogen is shown to activate the oxygen molecule and facilitate the above reaction. Moreover, impurity atoms of varying electronegativity has been introduced into pristine gold cluster to gain insight into the factors affecting CO oxidation reaction on these clusters and design better catalysts by modulating their electronic properties significantly. In the final part of this chapter, complexes of DNA base with gold clusters are shown as promising nanostructure for efficient CO oxidation process. Chapter 6 deals with several nanomaterials which assume importance in energy applications related to water splitting and hydrogen storage. This chapter begins with the investigations of water dissociation process on unsupported gold cluster as well as cluster supported on carbon nanostructures. It has been demonstrated that a gold cluster on a defective CNT can bring down barrier for water dissociation as compared to its unsupported counterpart. Another nanostructure, Ti decorated BN nanotube is also explored for its possible role in water dissociation process and generation of hydrogen molecule. In the concluding part of this chapter, hydrogen adsorption in Si-Li binary clusters have been investigated. The thesis concludes with chapter 7, where the possible future explorations of the present work have been discussed.

Publications

1. Naresh K. Jena, K. R. S. Chandrakumar, and Swapan K. Ghosh, "Theoretical Investigation on the Structure and Electronic Properties of Hydrogen- and Alkali-Metal- Doped Gold Clusters and Their Interaction with CO: Enhanced Reactivity of Hydrogen- Doped Gold Clusters", *J. Phys. Chem. C* 2009, *113*, 17885-17892.

2. Naresh K. Jena, K. R. S. Chandrakumar, and Swapan K. Ghosh, "Beyond the goldhydrogen analogy: Doping gold cluster with H-atom - O2 activation and reduction of reaction barrier for CO oxidation", *J. Phys. Chem. Lett.* 2011, *2*, 1476-1480.

3. Naresh K. Jena, K Srinivasu and Swapan K Ghosh, "Computational investigation of hydrogen adsorption in silicon-lithium binary clusters", *J. Chem. Sci.* 2012, *124,* 255- 260.

4. Naresh K. Jena, Manoj K. Tripathy, K. R. S. Chandrakumar, Alok K Samanta, and Swapan K. Ghosh, "Water molecule encapsulated in carbon nanotube model systems: Effect of confinement and curvature", *Theor. Chem. Acc.* 2012, *131*, 1205.

5. Naresh K. Jena, Mahesh Sundarajan, and Swapan K. Ghosh, "On the Interactions of Uranyl with Functionalized Fullerenes: A DFT investigation" *RSC Advances* 2012, *2*, 2994–2999.

6. Naresh K. Jena, K. R. S. Chandrakumar, and Swapan K. Ghosh, "DNA Base-GoldNano Cluster Complex as a Potential Catalyzing Agent: An Attractive Route for CO Oxidation Process" *J. Phys. Chem. C* 2012, *116*, 17063-17069.

7. Naresh K. Jena, K. R. S. Chandrakumar, and Swapan K. Ghosh, "Water Dissociation on Gold Cluster: Effect of Carbon Nanostructures as Substrate" *RSC Advances* 2012, doi:10.1039/C2RA21032K.

8. K. Srinivasu, Naresh K. Jena, and Swapan K. Ghosh, "Electronic structure, Stability and Non-linear Optical Properties of Aza-fullerenes C60-2nN2n(n=1-12)", (Submitted to *AIP Advances* 2012)

9. Naresh K. Jena, K. R. S. Chandrakumar, and Swapan K. Ghosh, "Governing Role of Nanoscale Curvature on the Electronic Properties and Reactivity of Carbon Nanotubes", (To be Submitted).

10. Naresh K. Jena, K. R. S. Chandrakumar, and Swapan K. Ghosh, "Dissociation of Water on a Ti-decorated BN Nanotbe: Insights from DFT Study", (To be Submitted).

11. Naresh K. Jena, K. R. S. Chandrakumar, and Swapan K. Ghosh, "Guiding Principles for CO oxidation on Gold Clusters", (To be Submitted).

Name	:	**Alok Rout**
Enrolment No.	:	CHEM02200704006
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	Computational Investigations on the Structure and Reactivity of Nanomaterials

Abstract

The work reported in the thesis involved the synthesis of various ionic liquids ranging from imidazolium to quaternary ammonium salts, amide and phosphonate functionalized ionic liquids and ionic liquids containing 1, 3-diketonate, alkylphophate and diglycolamate anions etc and using them for the separation of actinides and fission products from nitric acid medium. The diluent and extractant properties of ionic liquids were exploited by using hydrophobic ionic liquids in conjunction with the molecular extractant (CMPO – TBP, diamide, alkylphophsoric acid, diglycolamic acid etc.) and task specific ionic liquids (or functionalized ionic liquids). The extraction behavior of the metal ions in ionic liquid medium was studied in detail and the trend was compared with that of the conventional diluents systems to bring out the uniqueness of IL diluents. Remarkably higher distribution ratios and high selectivities were obtained for the metal ions when ionic liquid was used as diluent as compared to conventional diluents (e.g., n-DD). The third phase formation phenomenon usually encountered in conventional TRUEX solvent (0.2 M CMPO – 1.2 M TBP/n-DD) at high metal loadings could be avoided using ionic liquid as diluents.

Excellent separation of Eu(III) from Am(III) was observed in ionic liquid medium in conjunction with acidic extractants namely, di-2-(ethylhexyl) phosphoric acid (DEHPA) and bis-2-(ethylhexyl)dyglycolamic acid (HDEHDGA) respectively. This opens avenues for studying the Ln-An separation from high level liquid waste using ionic liquids. In all the above cases, imidazole based ionic liquids, 1-alkyl-3-methylimidazolium bis (trifluoromethanesulfonyl) imide ($C_n$mimNTf$_2$; n = 4, 5, 6, 8) were used as diluents.

Under the tasks specific ionic liquid category (TSIL), phosphonate and amide moienties were covalently grafted onto the imidazolium cation and the extraction studies were carried out. The results indicated unusual separation of Pu(IV) from other actinides and fission products while using TSILs.

New ionic liquids with 1, 3-diketonale, alkyl phosphate and diglycolamate anions which are very highly soluble in molecular diluents such as aromatics and normal paraffins were synthesized and studied for the extraction of Pu(IV) and Eu(III) from nitric acid medium.

Publications

1. Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Extraction of americium(III) from nitric acid medium by CMPO-TBP extractants in ionic liquid diluent. *Radiochim. Acta 97(12) (2009) 719-725.*

2. A. Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Unusual extraction of plutonium(IV) from uranium(VI) and americium(III) using phosphonate based task specific ionic liquid. *Radiochim. Acta 98 (8) (2010) 459 - 466.*

3. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Extraction and third phase formation behavior of Eu(III) in CMPO - TBP extractants present in room temperature ionic liquid. *Sep. Purif. Technol. 76 (3) (2011) 238 – 243.*

4. A. Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Ionic liquid extractants in molecular diluents: Extraction behavior of plutonium (IV) in 1, 3- diketonate ionic liquids. *Solvent Extr. Ion Exch. 29 (4) (2011) 602 – 618.*

5. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Room temperature ionic liquid diluent for the mutual separation of europium (III) from americium (III). *Sep. Purif. Technol. 81(2) (2011) 109 – 115.*

6. A. Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Room temperature ionic liquid diluent for the extraction of Eu(III) using TRUEX extractants. *J. Radioanal. Nucl. Chem. 290 (2011) 215 – 219.*

7. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Extraction behavior of actinides and fission products in amide functionalized ionic liquid. *Sep. Purif. Technol. DOI; 10.1016/j.seppur.2012-01.020.*

8. A. Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Separation of plutonium(IV) from uranium(VI) using phosphonate based task specific ionic liquid. *Desalination and water treatment. DOI: 10/5004/dwt.2012.2301.*

9. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Liquid – Liquid extraction of Pu(IV), U(VI) and Am(III) using malonamide in room temperature ionic liquid as diluent. *J. Hazard. Mater. (In Press).*

10. P. R. Vasudeva Rao, K. A. Venkatesan, Alok Rout, K. Nagarajan, T. G. Srinivasan, Potential Applications of Room Temperature Ionic Liquids for fission products and actinides separation. *Sep. Sci. and Technol. 47 (2012) 204–222.*

11. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Ionic liquid extractants in molecular diluents: II. Extraction behavior of europium (III) in quarternary ammonium-based ionic liquids. *Solvent Extr. Ion Exch. (Under review).*

B. Conferences and symposia papers

I. International

1. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao. Extrcation behavior of actinides and fission products using amide functionalized ionic liquid. 1st international conference on ionic liquids in separation and purification technology, ILSEPT, Sitges, Spain, 4th – 7th sep., 2011 (Given a Key note lecture and Chaired a session).

2. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao. Extraction behavior of Eu(III) in CMPO-TBP-Ionic liquid system, 2nd International conference on application of radioisoptopes in chemical, environmental and biological science, ARCEBS 2010, Saha Institute of Nuclear physics, Bidhan Nagar, Kolkata, India, November 7 – 13, 2010.

3. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao. Unusual miscibility of ionic liquid in paraffinic diluents. International Conference on Vistas in Chemistry (ICVC 2011), Oct 11 – oct 13, 2011, IGCAR, India.

II. National

1. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao. Extraction and stripping of Neodymium (III) and Dysprosium (III) by TRUEX solvent. Nuclear and Radiochemistry Symposium, NUCAR 2009, SVKM Mithibai College, Vile Parle, Mumbai, India, January 7-10, 2009.

2. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao. Comparison in the extraction behavior of Am(III) from nitric acid medium by TRUEX extractants in molecular and ionic liquid diluent. Emerging Trends in Separation Science and Technology, SESTEC 2010, Indira Gandhi Centre for Atomic Research, Kalpakkam, India, March 1-4, 2010 (Best Paper award).

3. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao. Separation of Plutonium(IV) from Uranium(VI) by Phosphonate based Task specific Ionic Liquid. Emerging Trends in Separation Science and Technology, SESTEC 2010, Indira Gandhi Centre for Atomic Research, Kalpakkam, India, March 1-4, 2010.

4. Alok Rout, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao. Extraction behavior of Pu(IV) by 1,3-diketonate based ionic liquid. Nuclear and Radiochemistry Symposium, NUCAR 2011, GITAM University, Visakhpatanam, India, February 22 – 26, 2011.

Name	:	**Satyanarayan Mukhopadhyay**
Enrolment No.	:	PHYS08200605005
Constituent Institute	:	Harish-Chandra Research Institute, Allahabad
Title	:	New Physics with Low Missing Energy: Identification and Discrimination at the LHC

Abstract

One of the most important goals of the Large Hadron Collider (LHC) is to probe new physics beyond the Standard Model (SM) of elementary Particles. One distinguishing criterion for new physics, often used in these searches, is a large amount of missing transverse energy, carried away by stable massive particles. However, this criterion may not be fulfilled in a number of well-motivated theoretical scenarios. We have considered several such situations, their characteristic signatures in the form of multiple leptons, and the criteria for distinguishing among various scenarios of this kind. We elaborate on the specific studies included in the thesis in the following.

In the presence of the T-parity violatingWess-Zumino-Witten (WZW) anomalyterm, the otherwise stable heavy photon in the Littlest Higgs model with Tparity (LHT) decays to either Standard Model gauge boson pairs, or to SM fermions via loop diagrams. We make a detailed study of the collider signatures where the heavy photon can be reconstructed from invariant mass peaks in the opposite sign same flavour dilepton or the four-lepton channel. This enables us to obtain information about the fundamental symmetry breaking scale in the LHT and thereby the low-lying mass spectrum of the theory. In addition, indication of the presence of the WZW term gives us hints of the possible UV completion of the LHT via strong dynamics.

In two subsequent studies, we point out that same-sign multilepton events, not given due attention yet for new physics search, can be extremely useful at the LHC. After showing the easy reducibility of the standardmodel backgrounds,we demonstrate the viability of same-sign trilepton (SS3ℓ) signals for R-parity breaking supersymmetry, at both 7 and 14 TeV LHC. We find that same-sign four-leptons (SS4ℓ), too, can have appreciable rates. In addition, we show how SS3ℓ and SS4ℓ, in conjunction with the mixed-sign trilepton and four-lepton channels, can be used to extract dynamical information about the underlying SUSY theory, namely, the Majorana character of the decaying lightest neutralino and the nature of L-violating couplings.

 This thesis also includes a study on the so-called LHC inverse problem. The problem of discriminating possible scenarios of TeV scale new physics with large missing energy signature at the LHC has received some attention in the recent past. We consider the complementary, and yet unexplored, case of theories predicting much softer missing energy spectra. As there is enough scope for such models to fake each other by having similar final states at the LHC, we have outlined a systematic method based on a combination of different kinematic features which can be used to distinguish among different possibilities. These features often trace back to the underlying mass spectrum and the spins of the new particles present in these models. As examples of "low missing energy look-alikes", we consider Supersymmetry with R-parity violation, Universal Extra Dimensions with both KK-parity conserved and KK-parity violated and the Littlest Higgs model with T-parity violated by theWess-Zumino-Witten anomaly term. Through detailed Monte Carlo analysis of the four and higher lepton final states predicted by these models, we show that the models in their minimal forms may be distinguished at the LHC, while non-minimal variations can always leave scope for further confusion.

Publications

(This thesis is based on the papers marked with an asterisk.)

* 1. *Dilepton and Four-Lepton Signals at the LHC in the Littlest Higgs Model with T-parity Violation* Satyanarayan Mukhopadhyay, Biswarup Mukhopadhyaya, Andreas Nyffeler Published in JHEP 1005:001,2010

* 2. *Same-sign trileptons and four-leptons as signatures of new physics at the Large Hadron Collider* Biswarup Mukhopadhyaya, Satyanarayan Mukhopadhyay Published in Phys.Rev.D82:031501,2010 (Rapid Communications).

* 3. *Discrimination of low missing energy look-alikes at the LHC* Kirtiman Ghosh，SatYanaraYan Mukhopadhyay, BiswarupMukhopadhyaya Published in JHEP 1010:096,2010

* 4. *Same-sign trileptons at the LHC: A Window to lepton-number violating super- symmetry* Satyanarayan Mukhopadhyay, Biswarup Mukhopadhyaya Published in Phys.Rev.D84:095001,2011

* 5. *Low-scale SUSY breaking by modular fields and Higgs mass bounds* Satyanarayan Mukhopadhyay, Biswarup Mukhopadhyaya, Soumitra Sen- Gupta E-print: arXiv:1103.3678 [hep-ph] 6. *Re-analysing the implications of CPT and unitarity for baryogenesis and lepto- genesis* Atri Bhattacharya, Raj Gandhi, Satyanarayan Mukhopadhyay E-print: arXiv:1109.1832 [hep-ph]

Name	:	**Sanjaykumar Hansraj Amrutiya**
Enrolment No.	:	MATH08200604006
Constituent Institute	:	Harish-Chandra Research Institute, Allahabad
Title	:	On Tannakian Fundamental Group Scemes, and On Real
		Parabolic Vector Bundles Over A Real Curve

Abstract

This thesis is divided into two parts.

In the first part, we consider Frobenius-finite vector bundles on an arbitrary pointed smooth projective variety (X, x) over a perfect field k of prime characteristic. Using these bundles, we construct a neutral Tannakian category CF (X) over k. By a well-known theorem, there is an affine group scheme over associated to C_F (X). This group scheme will be denoted by π_F (X, x), and is called the F-fundamental group scheme of (X; x). We study the properties of this affine group scheme.

In the second part, we define parabolic structures on real vector bundles over a real curve. Let (X, σ_X) be a real algebraic curve, and let S C X be a non-empty finite subset of X such that σ_X (S) = S. Let N $\geq$ 2 be an integer. We construct an N-fold cyclic cover p : $Y \rightarrow X$ in the category of real curves, ramified precisely over each point of S, and with the property that for any element g of the Galois group of Γ of p, and y ε Y , one has σ_Y (gy) = $g^{-1}\sigma_Y$ (y). The main theorem in this part gives an equivalence between the category of real parabolic vector bundles over X with parabolic structure over S, all of whose weights are integral multiples of $1=N$, and the category of Γ-equivariant real vector bundles over Y .

Publications

1. Sanjay Amrutiya, Indranil Biswas On the F-fundamental group scheme, Bull. Sci. \math. 134 (2010) 461-474.

2. Sanjay Amrutiya, On real parabolic vector bundles over a real curve, Preprint.

Name	:	**Karuna Kara Mishra**
Enrolment No.	:	PHYS02200704018
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	Raman and Brillouin Spectroscopic Studies of Phase Transitions in Perovskite Ferroelectric Materials

Abstract

Compound ferroelectric, relaxor ferroelectric and magnetic ferroelectric (multiferroic) materials with Perovskite structure have been of interest both from fundamental as well as applications point of view. This thesis reports Raman and Brillouin spectroscopic investigations of phase transitions in one representative system of each type: (a) ferroelectric $NaNbO_3$, (b) relaxor-ferroelectric $Pb(Zn_{1/3}Nb_{2/3})_{0.85}Ti_{0.15}O_3$ (PZN-PT) and (c) multiferroic $(Bi_{1-x}La_x)_{0.5}Pb_{0.5}Fe_{0.5}Ti_{0.5}O_3$, $0 \leq x \leq 0.5$ (BLF-PT). Temperature is used as a primary thermodynamic parameter to take the system across phase transition(s). Where ever possible, both polycrystalline ceramic samples and single crystals are investigated. In the case of BLF-PT, tetragonal-cubic structural transition induced by La-composition as well as by temperature is studied using *in-situ* high temperature X-ray diffraction. Supporting dielectric and magnetic measurements are also carried out, where ever necessary and correlation of these properties to structural changes are discussed. Ceramic samples of $NaNbO_3$ and BLF-PT were synthesized using solid reaction method. Single crystal of $NaNbO_3$ and PZN-PT were grown using flux method.

Low temperature Raman spectroscopic study on $NaNbO_3$ was carried out to investigate coexistence of anti-ferroelectric and ferroelectric phases. From the temperature dependence of intensities of modes characteristic of each phase a coexistence range of ~60 K and a hysteresis of ~80 K were found. A Brillouin spectroscopic study of the behavior of central peak parameters such as relaxation time and integrated intensity in $NaNbO_3$ single crystal as function of temperature across the antiferroelectric ($D_{2h}^{11}, Z = 8$) to antiferroelectric ($D_{2h}^{13}, Z = 24$) transition ~643 K suggested the transition to be order-disorder type. In relaxor PZN-PT single crystal a coupling between strain and polarization fluctuation was concluded from the behavior of relaxation times obtained from Brillouin study of LA phonon and central peak. The LA mode frequency and its line-width as a function of temperature showed anomalies across tetragonal-cubic phase transition ~463 K. Polarized Raman studies on PZN-PT single crystal also exhibit anomalies in the mode frequencies across the transition. BLF-PT was found to

undergo a tetragonal-cubic transition at a La composition of $x \geq 0.4$. A *x-T* phase diagram of BLF-PT was constructed based on *in-situ* high temperature X-ray diffraction results. From Raman spectroscopic study the phonons in the tetragonal phase were assigned and symmetry-forbidden Raman scattering in cubic phase was understood on the basis of substitutional disorder and compositional fluctuation. Magnetization as well as polarization properties were found to improve with decreasing lattice anisotropy (*c/a* - 1). For *x* = 0.2 system an Ising-type spin glass behavior was found.

Publications

1. Low-temperature Raman spectroscopic studies in $NaNbO_3$ K. K. Mishra, V. Sivasubramanian, and A. K. Arora, J. Raman Spectrosc. 42, 517 (2011).

2. Raman scattering from La-substituted $BiFeO_3$–$PbTiO_3$ K. K. Mishra, V. Sivasubramanian, R. M. Sarguna, T. R. Ravindran, and A. K. Arora, J. Solid State Chem. 184, 2381 (2011).

3. *x*-T phase diagram of La-substituted $BiFeO_3$-$PbTiO_3$ K. K. Mishra, R. M. Sarguna, S. Khan, and A. K. Arora, AIP Advances 1, 032126 (2011).

4. Vibrational, magnetic, and dielectric behavior of La-substituted $BiFeO_3$-$PbTiO_3$ K. K. Mishra, A. T. Satya, A. Bharathi, V. Sivasubramanian, V. R. K. Murthy, and A. K. Arora, J. Appl. Phys. 110, 123529 (2011).

5. Anomalous behavior of acoustic phonon mode and central peak in $Pb(Zn_{1/3}Nb_{2/3})_{0.85}Ti_{0.15}O_3$ single crystal studied using Brillouin scattering K. K. Mishra, V. Sivasubramanian, A.K. Arora, and D. Pradhan (Under review).

6. Brillouin spectroscopic study of central peak in $NaNbO_3$ single crystal K. K. Mishra, V. Sivasubramanian, A. K. Arora, and R. M. Sarguna (Under review).

7. Polarized *micro*-Raman spectroscopic study of relaxor $Pb(Zn_{1/3}Nb_{2/3})_{0.85}Ti_{0.15}O_3$ single crystal K. K. Mishra, V. Sivasubramanian, A. K. Arora, and D. Pradhan (Under review).

Publications not included in thesis

1. Impedance and Raman spectroscopic studies of $(Na_{0.5}Bi_{0.5})TiO_3$ B. K. Barick, K. K. Mishra, A. K. Arora, R. N. P. Choudhary, and D. Pradhan, J. Phys. D: Appl. Phys. 44, 355402 (2011).

2. Low Frequency Raman Scattering from Confined Acoustic Phonons in Free Standing Silver Nanoparticles Venu Mankad, K. K. Mishra, S. K Gupta, T.R. Ravindran, and P. K. Jha, J. Vibrational Spectrosc. 61, 183 (2012). Published Conference Proceedings

Published Conference Proceedings

1. Raman spectroscopic study of the coexistence of phases in $NaNbO_3$ K. K. Mishra, V. Sivasubramanian, and A.K. Arora Proc. 54th DAE Solid State Physics Symp. P. 159 (Boroda 2009).

2. Phonons in La-Substituted $BiFeO_3$-$PbTiO_3$ K.K.Mishra, V.Sivasubramanian, R.M.Sarguna, T.R.Ravindran, and A.K.Arora, Int. Conf. on Physics of Emerging Functional Material (Mumbai, 2010) AIP Conf. Proc. 1313, 174-176 (2011).

3. Magnetic ordering in La-substituted $BiFeO_3$-$PbTiO_3$ K. K. Mishra, A.T. Satya, A. Bharathi, and A. K. Arora, 56th DAE Solid State Physics Symp. (Chennai, 2011) AIP Conf. Proc. 1447, 1149-1150 (2012).

Conference papers – Unpublished (Abstract only)

1. Tetragonal-Cubic transition in multiferroic La-substituted $BiFeO_3$-$PbTiO_3$ K. K. Mishra, R. M. Sarguna, and A. K. Arora National Conf. on Recent Trends in Material Science (Wakanaghat, 2011).

Name	:	**Sreejith Kaniyankandy**
Enrolment No.	:	CHEM01200604009
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Charge Transfer Dynamics in Quantum Dot & Quantum Dot Based Nanostructures

Abstract

The present thesis deals with charge carrier dynamics in quantum dot based nanostructures. It is aimed at understanding how; under defined regime the dynamic properties are affected. The investigated nanomaterials are TiO_2, II-VI semiconductor based QD and QD core/shell nanomaterials.

The thesis describes how small nanostructures are different from their bulk counterparts, in terms of electronic structure. Additionally how this electronic structure influences dynamic properties is also discussed. In a TiO_2 nanostructure this has been has been demonstrated using an excited absorbate to inject electrons in QD (TiO_2) and also by studying size dependent dynamics properties of nanostructures (CdTe). These studies on charge carrier dynamics have been carried out by using femtosecond transient absorption spectroscopy. These dynamical properties were found to be influenced by both the change in electronic structure and also due to an uncoordinated or a defected surface.

Another nanostructure we investigated was CdTe-Reduced Graphene Oxide nanocomposite. Significant reduction in charge recombination was observed in this tailor made system indicating an efficient charge separation.

Furthermore, dynamics in novel nanostructures like core shell (CdSe/ZnTe core shell) are also investigated. Here we aimed at understanding how fast a charge transfer process occurs via interface from one semiconductor to other by monitoring the exciton bleach dynamics of one of the semiconductors.

A major portion of study also involved synthesis of novel nanostructures.

The present thesis illustrates different ways one can employ to achieve a better charge separation. The approaches illustrated not only using single nanostructure but also composites and core shell geometry to achieve this purpose.

Publications

1. Efficient Charge Separation in CdTe Quantum Dot decorated Graphene. Sreejith Kaniyankandy, Sachin Rawalekar, and Hirendra N. Ghosh, *Journal of Physical Chemistry C, 116*, 16271–16275 (2011)

2. Ultrafast Relaxation Dynamics in Graphene Oxide: Evidence of Electron Trapping, Sreejith Kaniyankandy, S. N. Achary, Sachin Rawalekar, and Hirendra N. Ghosh, *Journal of Physical Chemistry C, 115*, 19110–19116 (2011)

3. Ultrafast Hole Transfer in CdSe/ZnTe Type II Core-Shell Nanostructure, Kaniyankandy, S., Rawalekar, S.,Verma, S., Ghosh, H. N., *Journal of Physical Chemistry C,*115, 1428-1435 (2011)

4. Charge Carrier Dynamics in Thiol Capped CdTe Quantum Dots, Kaniyankandy, S., Rawalekar, S.,Verma, S., Palit, D. K. *Physical Chemistry Chemical Physics* 12, 4210-4216 (2010).

5. Efficient Luminescence and Photocatalytic Behavior in Ultrafine TiO2 Particles Synthesized by Arrested Precipitation, Kaniyankandy, S., Ghosh, H. N. *Journal of Materials Chemistry*, 19, 3523-3528 (2009

6. Evidence of Multiple Electron Injection and Slow Back Electron Transfer in Alizarin-Sensitized Ultrasmall TiO2 Particles, Kaniyankandy, S., Verma, S., Mondal, J. A., Palit, D. K., Ghosh, H. N. *Journal of Physical Chemistry C* 113, 3593-3599 (2009)

Name   :   **Jatish Kumar Dash**
Enrolment No.   :   PHYS07200604036
Constituent Institute   :   Institute of Physics, Bhubeneswar
Title   :   Growth of Si-Ge Nanostructures on High Index Silicon Surfaces
                                             using Molecular Beam Epitaxy and their Characterizations

Abstract

The thesis reports the shape evolution of Si-Ge nanostructures on various high index silicon
Surfaces, grown by molecular beam epitaxial (MBE) under ultra-high vacuum (UHV) conditions. The morphological dynamics have been analyzed in different thermodynamic growth conditions and substrate orientations. A comparative study of the Si-Ge structures on the reconstructed high index surfaces, such as, Si(5 5 12), Si(5 5 7) and (5 5 3), has been presented in terms of shape transformations with varying growth coverage, substrate temperature and mode of annealing conditions. In the first part of the thesis work, we show that self-assembled growth at optimum thickness of the over layer leads to interesting shape transformations, namely, from nanoparticle to trapezoidal structures at higher thickness values. Thin films of Ge of varying thickness form 3 to 10 monolayer (ML) were grown under ultra-high vacuum conditions on a Si(5 5 12) surface at a substrate temperature of 600^0C. The substrate heating was achieved by two methods: (i) by heating a filament under the substrate (radiative heating, RH) and (ii) by passing direct current (DC) through the samples in three directions (perpendicular, parallel and at 45^0 to the step direction $<110>$. We found irregular, spherical island structures under RH conditions. The shape transformations have been found under DC heating conditions and for Ge deposition more than 8 ML thick. Well aligned trapezoid structures are found along $<110>$ irrespective of the DC current direction. Also we observe the absence of such a shape transformation in the case of Ge deposition on low index surface like Si(111). Scanning transmission electron microscopy (STEM) measurements suggested the mixing of Ge and Si. This has been confirmed with a quantitative estimation of the intermixing using high resolution X-ray diffraction (HRXRD) and Rutherford backscattering spectrometry (RBS) measurements.

A comparative study on the shape evolution of MBE grown $Si_{1-x}Ge_x$ islands on ultraclean reconstructed high index Si(5 5 12), Si(5 5 7) and Si(5 5 3) surfaces has been carried out experimentally and explained using a phenomenological kinetic Monte Carlo (kMC) simulation.

We observe universality in the growth dynamics in terms of aspect ratio and size exponent, for all three high index surfaces, irrespective of the actual dimentions of Ge-Si structures. The shape evolution has been simulated using kMC by introducing a deviation parameter (ε) in the surface barrier term (E_D) to take the effect of anisotropic diffusion, as one of the plausible mechanisms. To see the effect of substrate temperature during growth, a temperature dependent shape evolution study was carried out. The morphological evolution and the effect of growth temperature on size, orientation and composition of molecular beam epitaxy grown Ge-Si islands on Si(5 5 12) surfaces have been investigated in the temperature range from room temperature (RT) to 800^0C. In the RH case, we found spherical island st 600^0C with a bimodal distribution and upon increasing temperature, the structures got faceted at 700^0C. At 800^0C thick dome like structures are formed bounded by facet planes. While in the case of DC heating, after the optimum critical temperature 600^0C, well aligned trapezoidal $Si_{1-x}Ge_x$ structures with a graded composition starts forming along the step edges. Interestingly, these aligned structures have been found only 600^0C, neither at low temperature nor at higher temperatures.

Publications

1. Universality in shape evolution of Si1–xGex structures on high index Silicon surfaces J. K. Dash, T. Bagarti, A. Rath, R. R. Juluri, P. V. Satyam Submitted to Eur. Phys. Lett., arXiv:1204.0578v1 (2012)(Under review).

2. Growth of Oriented Au Nanostructures: Role of Oxide at the Interface A. Rath, J. K. Dash, R. R. Juluri, A. Rosenauer, Marcos Schoewalter and P. V. Satyam J. Appl. Phys. 111, 064322 (2012).

3. DC heating induced shape transformation of Ge structures on ultra clean Si (5 5 12) surfaces J. K. Dash, A. Rath, R. R. Juluri, P. Santhana Raman, K. Muller, A. Rosenauer and P. V. Satyam J. Phys.: Condens. Matter 23, 135002 (2011).

4. Shape transformation of Si1–xGex structures on ultra clean Si (5 5 7) and Si (5 5 12) surfaces J. K. Dash, A. Rath, R. R. Juluri, K. Mueller, A. Rosenauer, P. V. Satyam J. Phys: Conf. Series 326, 012021 (2011).

5. Nano scale phase segregation and alloy formation in Au-Ge system on ultra clean surfaces A. Rath, J. K. Dash, R. R. Juluri, A. Rosenauer and P. V. Satyam J. Appl. Phys. 111, 104319 (2012).

6. Shape evolution of MBE grown Si1–xGex structures on high index Si(5 5 12) surfaces: A temperature dependent study J. K. Dash, A. Rath, R. R. Juluri, P. V. Satyam Submitted to J. Physics D: Appl. Phys.(Under review)(2012).

7. Compositional analysis of Aligned trapezoid Si-Ge structures on Si(5 5 12) surfaces J. K. Dash, A. Rath, R. R. Juluri, P. V. Satyam To be published (2012).

8. Temperature dependent electron microscopy study of Au thin films on Si(100) with and without native oxide layer as barrier at the interface A. Rath, J. K. Dash, R. R. Juluri, A. Rosenauer and P. V. Satyam J. Physics D: Appl. Phys., 44, 115301 (2011).

9. Epitaxy-like orientation of nanoscale Ag islands grown on air-oxidized Si(110)- (5 × 1) surfaces Anupam Roy, J. K. Dash, A. Rath and B. N. Dev Surface and Interface Anlysis (wileyonlinelibrary.com) DOI 10.1002/sia.3837.

10. Growth of oriented Ag nanocrystals on air-oxidized Si surfaces: An insitu high energy electron diffraction study Anupam Roy, K. Bhattacharjee, J. K. Dash and B. N. Dev Thin Solid Films 520, 853-860 (2011).

11. Migration and extrusion of metal nanowire inside the filled multi-walled carbon nanotube Pawan K. Tyagi, Umananda M. Bhatta, Ashutosh Rath, J. Raghavendra Rao, Jatis K. Dash, Sanjeev Kumar, and P. V. Satyam Submitted to Carbon (2012).

12. Observation of grain growth in swift heavy ion irradiated NiO thin films P. Mallick, Chandana Rath, J. K. Dash, R. Biswal, D. C. Agarwal, D. Behera, D. K. Avasthi, D. Kanjilal, P. V. Satyam and N. C. Mishra Ind. J. Phys. 84 (10), 1399-1404 (2010).

13. Formation of aligned nano-silicide structures in MBE grown Au/Si(110) system: A real time temperature dependent TEM study Umananda M. Bhatta, J. K. Dash, Anupam Roy, A. Rath and P. V. Satyam J. Phys.: Condens. Matter 21 ,205403 (2009)

14. Real time study of oxide mediated liquid - solid growth of high aspect ratio - aligned gold silicide microrods on Si (110) substrates Umananda M. Bhatta, Ashutosh Rath, Jatis K. Dash, Jay Ghatak, Lai Yi-Feng, Chuan-Pu Liu, P. V. Satyam Nanotechnology 20, 465601 (2009).

15. Structural phase transitions in Au thin films on Si (110): An in-situ temperature dependent transmission electron microscopy study Umananda M. Bhatta, J. K. Dash, A. Rath, P. V. Satyam Appl. Surf. Sci., 256, 567 (2009).

16. Growth of oriented crystalline Ag nanoislands on air-exposed Si(001) surfaces A. Roy, K. Bhattacharjee, J. K. Dash and B. N. Dev Appl. Surf. Sci., 256, 361(2009).

Conference Presentations

1. Shape transformation of Si1–*x*Ge*x* structures on ultra clean Si (5 5 7) and Si (5 5 12) surface J. K. Dash, A. Rath, R. R. Juluri, K. Mueller, A. Rosenauer, P. V. Satyam Microscopy of Semiconducting Materials, MSM-2011, Churchill College, Cambridge, UK.

2. Shape Evolution of MBE Grown Si1–*x*Ge*x* Structures on High Index Silicon Surfaces: A Temperature Dependent Study J. K. Dash, A. Rath, R. R. Juluri, P. V. SatyamICANN-2011, Indian Institute of Technology Guwahati (IITG).

3. Poster pressentation at Workshop on Elecron Microscopy (WEM-2011) held at Institute of Physics, Bhubaneswar, India.

4. Presented a poster in International conference on Ion beam induced nanopatterning of materials (IINM-2011), Institute of Physics, Bhubaneswar, India.

5. Oral presentation at Seminar on Physics and Technology of Novel Materials (PTNM-2010) at Sambalpur University,Sambalpur, Odisha, India.

6. Poster presentation at International Conference on Physics at Surfaces and Interfaces, PSI-2009, Toshali Sands, Puri, India.

Name	:	**Prabal Singh Verma**
Enrolment No.	:	PHYS06200704011
Constituent Institute	:	Institute of Plasma Research, Gandhinagar
Title	:	Study of Nonlinear Oscillations and Waves in Plasma

Abstract

In this thesis we studied nonlinear oscillations/waves in a cold plasma in various physical limits and investigated several novel aspects of wave breaking which have not been considered up till now. We have obtained an exact solution in the lab frame describing the space time evolution of an arbitrary perturbations in a cold homogeneous plasma and have shown that addition of a second harmonic increases the breaking amplitude of the fundamental mode. Later we verified this interesting observation in 1-D particle in cell simulation. We have further studied nonlinear oscillations in a cold viscous/hyperviscous and resistive plasma and obtained an expression describing the breaking criterion for Dawson like perturbation [102] for this case. Moreover, we have shown that the nonlinear effects as reported in a recent reference are independent of the model for viscosity chosen in the ref. [118]. We have numerically studied the breaking criterion of longitudinal AkhiezerPolovin (AP) waves [119] in the presence of noise and found that they break at arbitrarily low amplitude through the process of phase mixing. Moreover, we have obtained longitudinal AP wave solution [119] from space time dependent solution of relativistic electron fluid equations for the cold homogeneous plasma [107]. We have also shown that it is not only the nonlinearly driven ponderomotive forces but the naturally excited zero frequency mode of the system may also be responsible for the phase mixing in an arbitrary mass ratio cold plasma. For example we have shown that the BGK waves in a cold electron plasma phase mix away and break at arbitrarily small amplitude via phase mixing if we allow ions to move. Here zero frequency mode of the system is found to be the only candidate responsible or phase mixing. We have also shown that there exist nonlinear traveling wave solutions in an arbitrary mass ratio cold plasma which do not exhibit phase mixing. Further, we have studied electron plasma oscillations beyond wave breaking using 1-D particle in cell simulation and found that a fraction of energy, decided by Coffey's limit in warm plasma [121], always remains with the wave in the form of the superposition of two BGK waves. This result is in contrast to the accepted fact that after the wave breaking all energy of the wave goes to random kinetic energy of the particles [102, 122]. The final distribution function is found to be non-Maxwellian. Lastly we studied development and collapse of double layers in the long scale length limit using method of Lagrange variables.

Publications

1. Residual Bernstein-Greene-Kruskal-like waves after one-dimensional electron wave breaking in a cold plasma _, Prabal Singh Verma, Sudip Sengupta, and Predhiman Kaw Phys. Rev. E 86, 016410 (2012)

2. Breaking of Longitudinal Akhiezer-Polovin Waves _, Prabal Singh Verma, Sudip Sengupta, and Predhiman Kaw Phys. Rev. Lett. 108, 125005 (2012)

3. Bernstein-Greene-Kruskal waves in relativistic cold plasma _, Prabal Singh Verma, Sudip Sengupta, and Predhiman Kaw Phys. Plasmas 19, 032110 (2012)

4. Nonlinear oscillations and waves in an arbitrary mass ratio cold plasma _, Prabal Singh Verma Phys. Plasmas 18, 122111 (2011)

5. Nonlinear evolution of an arbitrary density perturbation in a cold homogeneous unmagnetized plasma _,Prabal Singh Verma, Sudip Sengupta, and Predhiman Kaw Phys. Plasmas 18, 012301 (2011).

6. Nonlinear oscillations in a cold dissipative plasma Prabal Singh Verma, J. K. Soni, Sudip Sengupta, and Predhiman Kaw Phys. Plasmas 17, 044503 (2010)

7. Spatio-temporal evolution and breaking of Double layers: A description using Lagrangian hydrodynamics, Predhiman Kaw, Sudip Sengupta, and Prabal Singh Verma submitted

Name   :   **Jaban Meher**
Enrolment No.   :   MATH08200604010
Constituent Institute   :   Harish-Chandra Research Institute, Allahabad
Title   :   Some Problems on Modular Forms

Abstract

We discuss some properties of the exponents of q-product expansions of certain class of generalized modular functions on the Hecke congruence subgroup of level N. We prove that under certain conditions on the generalized modular function, the exponents $c(p)$ (p prime) of the q-product expansion of a generalized modular function take infinitely many different values. We also show that under the hypothesis that the divisor of a generalized modular function is empty, the exponents $c(n)$ (n>0) change signs infinitely often, provided that $c(n)$ are real numbers.

Next, we discuss about the theory of newforms of half-integral weight. We set up the theory of newforms for both Kohnen plus space and the full space on the space of cusp forms of level 8N and 16N, where N is a square-free positive integer. We use the isomorphism between the space of halfintegral weight cusp forms and integral weight cusp forms, given by M. Ueda to develope themtheory. We also prove a Waldspurger type result relating the Fourier coefficients of a half-integral modular form and value of L-function at the center associated to the corresponding integral weight modular form under the Shimura correspondence for the Kohnen plus space of level 8N.

It is known that except for finitely many explicit cases, the product of two eigenforms is not an eigenform. We generalize this result to other kinds of modular forms. Namely, we investigate the cases for which products of two quasimodular or nearly holomorphic eigenforms are eigenforms.

We also generalize the results on products of eigenforms of higher levels to the case of Rankin-Cohen brackets.

Publications

1. [KM] W. Kohnen and J. Meher, some remarks on the q-exponents of generalized modular functions, Ramanujan J. 25 (2011), no. 1, 115-119.

2. [MMR] M. Manickam, J. Meher and B. Ramakrishnan, Newsforms of Half-integral weight on $\Gamma_0(8N)$ and $\Gamma_0(16N)$, preprint 2011.

3. [M] J. Meher, Some Remarks on Rankin-Cohen Brackets of Eigen forms, preprint 2011, arXiv:1111.2431.

Name	:	**Surendra Mishra**
Enrolment No.	:	PHYS01200904001
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Optimization Studies for Physics Problems in Indian PHWRs

Abstract

There are fifteen small sized 220 MWe Pressurized Heavy Water Reactors (PHWRs) and two medium sized 540 MWe PHWRs operating in India. The more advanced 700 MWe PHWRis in design stage and would be commissioned in near future. In this thesis, three types of core-level optimization problems relevant to Indian PHWRs have been studied.

The first problem is concerned with generation of fresh core loading pattern for initial fuel loading in PHWRs. If the full reactor core is loaded with fresh Natural Uranium (NU) bundles, the reactor cannot operate at full power because of high power peaking in central region. Hence, it is necessary to load few Thorium or Depleted Uranium (DU) bundles to flatten the power. The choice of best locations of Thorium or DU bundles is a very large-sized constrained combinatorial optimization problem which cannot be solved by brute force. The fuel loading has to be such that the reactor can operate at full power right from beginning without violating the limit on bundle power, channel power and reactivity worth in shutdown systems. This problem is solved in a novel way using Evolutionary Algorithms. Several suitable loading patterns for 220 MWe and 700 MWe reactors have been explicitly generated.

The second problem is concerned with the design of Thermal Power Monitoring System(TPMS) used to estimate bulk and zonal powers in 700 MWe PHWR. For this purpose, out of the total 392 fuel channel, 44 channels are instrumented. Choosing these 44 channels so as to maximize the power prediction accuracy is combinatorial optimization problem. This problem is solved using an Evolutionary Algorithm.

The third problem is concerned with the optimum choice of a computational method for on-line Flux Mapping System (FMS) in 700 MWe PHWRs. The FMS determines details neutron flux distribution using 102 in-core neutron detector readings. There exist many computational methods for this purpose. Four different methods are compared and an optimum method has been identified which gives good accuracy without too much computational effort. Many methods use higher K-modes as basis functions. Optimization of the number of models is also studied.

Publications

1. Surendra Mishra, R. S. Modak and S. Ganesan; "Optimization of Thorium loading in fresh core of Indian PHWR by evolutionary algorithms". Annals of Nuclear Energy 36 (2009), 948-955.

2. Surendra Mishra, R. S. Modak and S. Ganesan; "Optimization of depleted uranium bundle loading in fresh core of Indian PHWR by evolutionary algorithm". Annals of Nuclear Energy 37 (2010) 208-217.

3. Surendra Mishra, R. S. Modak and S. Ganesan; "Optimization of depleted uranium loading in fresh core of large sized Indian PHWR by evolutionary algorithm". Annals of Nuclear Energy 38 (2011) 905-909.

4. Surendra Mishra, R. S. Modak and S. Ganesan; "Selection of Fuel Channels for Thermal Power Measurement in 700 MWe Indian PHWR by evolutionary algorithm". *Manuscript Submitted to Nucl. Eng. Design on 6th May 2011 and is under review.*

5. Surendra Mishra, R. S. Modak and S. Ganesan; "Computational Schemes for Online Flux Mapping System in a large sized Pressurized Heavy Water Reactor". *Nuclear Science and Engineering 170 (2012), 280-289.*

B. Posters in Conferences / Internal Reports

1. Surendra Mishra, R. S. Modak, S. Ray, A.N. Kumar and S. Ganesan; "On the Optimization of Thorium Bundle Distribution in the initial core loading for a PHWR". International Conference on Peaceful Uses of Atomic Energy-2009, Sep.29- Oct. 1, 2009, New Delhi, India.

2. Surendra Mishra, Sherly Ray, A. S. Pradhan and A. N. Kumar; "Initial Fuel Loading for KAPS#1 using DDU Bundles". NPCIL Design Note No. KAPS-1,2/DN/01100/10014 dated 12 August 2010.

3. Surendra Mishra, Sherly Ray, A. S. Pradhan and A. N. Kumar; "Initial Fuel Loading Pattern for 700 MWe PHWR using DDU Bundles". NPCIL Design Note No. KAPP-3,4/DN/01100/10012 dated 29 September 2010

Name	:	**Umesh Kumar V. Dubey**
Enrolment No.	:	MATH08200604010
Constituent Institute	:	Institute of Mathematical Science, Chennai
Title	:	Some Problems on Modular Forms

Abstract

Given a quasi-projective scheme X with an action of a finite group G we consider the tensor triangulated category DG(X) . We relate the spectrum of this category, as defined by P. Balmer, with the spectrum of the category of all perfect complexes over the scheme X/G. Similarly, we consider the category of perfect complexes Dper(X) over a split super-scheme X. We give isomorphism of the spectrum of Dper(X) with the spectrum of Dper(X0). Here X0 denotes the even part of the super-scheme X ; it is a scheme in the usual sense. The computation of these two spectrums gives examples of two distinct categories with isomorphic Balmer spectrums. Our result also shows the limitations of the geometric notion spectrum beyond the category of schemes. We suggest some possible generalisations of Balmer's notion of spectrum.

Publications

1.   (with Vivek M. Mallick). Spectrum of some triangulated categories, ERA-MS, Vol. 18, 2011, 50- 53.

2.   (with Vivek M. Mallick). Spectrum of some triangulated categories, (submitted) arXiv:1012.0789.

Name	:	**Sumana Sengupta**
Enrolment No.	:	CHEM01200604007
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Gas-Phase Chemistry of Atmospherically Important Compounds

Abstract

Laser photolysis-laser induced fluorescence, was used for the kinetic study of reaction of OH radicals with Bis-trifluoroethylether ($CF_3CH_2OCH_2CF_3$(TFEE)), which is a chlorofluorocarbon alternative, and Morpholine, a polyfunctional compound (secondary amine/ cyclic ether) in the temperature range 298-365K. For TFEE, the bimolecular rate-coefficient (k_{II}) at 298K, was measured as $(1.47 \pm 0.3) \times 10^{-13}$ cm^3 molecule^{-1}S^{-1} , and the temperature dependence of k_{II} was $(4.5 \pm 0.8) \times 10^{-12}$exp[-(1030 ± 20)T] cm^3 molecule^{-1}S^{-1}. For morpholine, k_{II} at 298K was found to be $(0.8 \pm 0.03) \times 10^{-10}$ molecule^{-1}cm^{3}s^{-1}. The temperature dependence of k_{II} was $(1.1 \pm 0.1) \times 10^{-11}$ exp [(590 ± 20)/T] cm^{3}molecule^{-1}s^{-1}. Theoretical calculations, by Gaussian 92 revealed that, OH radical forms pre-reactive complex, by bonding with the N-,or O-, atom of morpholine, before H-abstraction.

OH radical was formed by photolysis of tetrahydrofuran (THF), tetrahydropyran(THP) and morpholine, which are cyclic ethers with interesting structural properties, and differently substituted epoxides, which are 3-memberd cyclic ethers, like butadienemonoxode (BMO) and styreneoxide (SO), by 193 nm laser. Dynamics studies revealed a complex reaction pathway, involving ring opening and intramolecular rearrangement. In the unsymmetrically substituted epoxides, the cleavage of the two different C—O bonds generated different biradicals, which underwent various reaction channels, the OH formation channel being most energy demanding as found by theoretical studies.

Publications

1. Kinetic study of the gas-phase reaction of hydroxyl radical with CF3CH2OCH2CF3 using LP-LIF method *International Journal of Chemical Kinetics 42 (2010) 519* S. SenGupta, Y. Indulkar, A. Kumar, and S. Dhanya

2. Kinetics of gas phase reaction of OH with morpholine – an experimental and theoretical study *The Journal Of Physical chemistry 114 (29) 7709* S. SenGupta, Y. Indulkar, A. Kumar, S. Dhanya, P.D. Naik, and P. N. Bajaj

3. Detection of OH radical in laser induced photodissociation of tetrahydrofuran at 193 nm *The Journal Of Chemical Physics 122 (2005) 124309* S. SenGupta, H. P. Upadhyaya, A. Kumar, P. D. Naik and P. N. Bajaj

4. Dynamics of OH radical generation in laser-induced photodissociation of tetrahydropyran at 193 nm *The Journal Of Chemical Physics 124 (2006) 024305* S. SenGupta, H. P. Upadhyaya, A. Kumar, P. D. Naik and P. N. Bajaj

5. The dynamics of OH generation by photodissociation of morpholine molecule at 193 nm *Chemical Physics Letters 465 (2008) 197–202* SenGupta, A. Kumar , P.D. Naik, and P.N. Bajaj

6. Detection of OH on photolysis of styrene oxide at 193 nm in gas phase *Chemical Physics Letters 430 (2006) 240–246* A. Kumar , S. SenGupta, K.K. Pushpa, P.D. Naik, P.N. Bajaj 214.

Name	:	**K. Tirumalesh**
Enrolment No.	:	CHEM01200604019
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Characterisation of Ground Water in the Coastal Aquifers of Pondicherry Region using Chemical Isotopic and Geochemical Modeling Approaches

Abstract

Coastal aquifers, which are typically characterized by variations in groundwater quality in space and time, are vulnerable directly and indirectly by anthropogenic activities and climate change induced sea water intrusion. Despite endowed with substantial water resources due to wide network of tanks, rivers and good rainfall, Pondicherry region demonstrates a drastic depletion of groundwater levels and contamination from manmade activities. This thesis work evaluates the groundwater quality and factors affecting their characteristics in potential water bearing zones with the help of geochemical, microbiological, environmental isotopic and modeling approaches covering three components viz., *groundwater*, *sediment* and *particles*.

Groundwater quality is fresh in most of the locations and suitable for drinking and agriculture purposes, however saline water ingression is noticed in the southeastern locations of the study area. No nitrate or fluoride contamination is observed but half of the samples analyzed indicate the presence of E. coli. Indicators such as SAR, RSC and Na% that qualify the water for irrigation suitability are found to be under 'excellent' to 'permissible' category. Major processes influencing groundwater chemistry are found to be dissolution of carbonate minerals, ion exchange and mixing of evaporated surface water. These results are further confirmed by environmental isotope trends. Tritium results indicate that groundwater is receiving modern recharge except in some deep Tertiary and Cretaceous zones. Sporadic incidences of arsenic are found in some deep groundwaters and the hydrochemical results suggest reductive dissolution as the governing process. The trace element and rare earth element ratios suggest that sediments are derived mainly from felsic source rocks. Arsenic content found increasing along the depth and TXRF analysis of sediment shows the presence of As in association with Fe and S.

The groundwater particle load ranges from 0.64 to 2.6 mg/L. A systematic decrease in particle number is observed with increasing well depth. The particle number is found to be influenced predominantly by organic carbon and ionic strength whereas pH and

temperature of the groundwater show negligible effect. Chemical analysis of the particles showed Na^+, K^+, Ca^{2+}, Mg^{2+} and iron elements and the source could be Feldspar, Carbonate and Ferromagnesium minerals that are present in sedimentary formations of this region. It is observed that Sr^{2+} preferential partitions in to colloidal over particulate matter as compared to Ca^{2+} and its transport is mainly as adsorbed species on clay bound particles.

Publications

1. Rare earth elements distribution in clay zones of sedimentary formation, Pondicherry, South India, K. Tirumalesh, K. L. Ramakumar, S. Chidambaram, S. Pethaperumal and Gursharan Singh, Journal of Radioanalytical and Nuclear Chemistry (10.1007/s10967- 011-1606-9).

2. An over view on NETPATH geochemical modeling- a case study from coastal aquifer of Pondicherry, K. Tirumalesh, K. L. Ramakumar, K. Shivanna, S. Chidambaram, Groundwater Monitoring and Management through Hydrogeochemical Modeling Approach, IK International Publishing House, New Delhi, march 2010, pp.33-47.

3. Occurrence of arsenic and its distribution in different sedimentary formations of coastal Pondicherry, India, K. Tirumalesh, K. L. Ramakumar, S. Chidambaram, Gursharan Singh and Pethaperumal, Applied Geochemistry (under review).

4. Microbial evaluation of groundwater from major sedimentary aquifers of Pondicherry region – insights into redox condition of the aquifer system, K. Tirumalesh, K. L. Ramakumar, S. Chidambaram, S. Pethaperumal, Gursharan Singh, D. Prakash, N. Nawani and M.V. Prasanna, Environmental Monitoring Assessment (under review).

5. A study on evolution of sedimentary deposits from coastal Pondicherry region using geochemical and isotope tools, K. Tirumalesh, S. Chidambaram, K. L. Ramakumar, U.P. Kulkarni, S. Pethaperumal, Gursharan Singh, Sedimentology (under review).

6. Evaluation of groundwater quality and its suitability for drinking and agricultural use in Pondicherry and its environs, South India, K. Tirumalesh, S. Chidambaram, K. L. Ramakumar, S. Pethaperumal, Gursharan Singh, Environmental Monitoring Assessment (under review).

7. Environmental isotopic constraints for the origin and residence time of groundwater from sedimentary aquifers of Pondicherry region (under preparation).

8. A study on evolution of groundwater geochemistry in coastal aquifers of Pondicherry region using statistical and geochemical modeling techniques (under preparation).

9. Role of colloidal particles in migration of strontium in deep groundwater – a case studyfrom Pondicherry region (under preparation).

International Conference / Symposium

1. K.Tirumalesh, K. L. Ramakumar, Gursharan Singh, S. Chidambaram, K. K. Swain, "Arsenic distribution in sedimentary formations of coastal Pondicherry, India – a case study", 2SM 2012.

2. K.Tirumalesh, K. L. Ramakumar, U.P. Kulkarni, Gursharan Singh, S. Chidambaram, "Source rock identification of sediments using trace element ratios and 13C isotope data – a case study from Pondicherry region", I2SM 2012. (Best Poster Award)

3. K.Tirumalesh, K. L. Ramakumar, Gursharan Singh, S. Chidambaram, R.K. Singhal, Manisha Venkatesh, "Strontium association with particulate matter in coastal groundwaters of Pondicherry, India", I2SM 2012.

4. K.Tirumalesh, Manoj Sharma, K.Shivanna and K.L. Ramakumar, Determination of arsenite at nanogram level in natural waters by anodic stripping differential pulse Voltammetry", 2nd International conference on Application of Radiotracers in Chemical, Environmental and Biological Sciences (ARCEBS-10), held in Kolkata during 7-13, November 2010., pp. 292-294.

5. K.Tirumalesh, K. Shivanna, K. L. Ramakumar, S. Chidambaram, "Implication of positiveEu anomaly in clay zones of sedimentary formation, Pondicherry, South India", FourthInternational Symposium on Nuclear Analytical Chemistry (NAC-IV), held in Mumbaiduring 15-19, Nov., 2010, pp. 277.

Name	:	**Tabish**
Enrolment No.	:	LIFE09200604007
Constituent Institute	:	Tata Memorial Centre, Mumbai
Title	:	Genotype Molecular Phenotype Correlation using Lymphoblastoid Cell Lines from Patients with Multiple Primary Neoplasms

Abstract

Advancement in diagnostic and treatment modalities has lead to improved disease management and increased survival of patients with carcinomas of upper aero-digestive tract (UADT). However this improvement has not been able to mitigate the development of second/ multiple primary neoplasm(s) (MPN) which now looms large at an annual risk of 3-7% in early stage UADT cancer survivors. In our previous study we demonstrated the ability of key SNPs in genes falling in major carcinogenesis pathways combined with tobacco usage iin predicting the incidence of tobacco related MPN. In this study, we genotyped 22 single-nucleotide polymorphisms (SNPs) in genes involved in DNA repair, apoptosis, cell cycle regulation and xenobiotic metabolism and created a genotype score (G score) from the number of variant alleles. The genotype was correlated with carcinogen sensitivity phenotype, quantified by Gamma radiation and benzo(a)pyrene diol epoxide (BPDE) induced cell cycle arrest, DNA damage/repair and percent cell death, using lymphoblastoid cell lines generated from UADT MPN patients (n=20) and healthy controls (n=10). The Distinctive polymorphism based G score signature was statistically different between the two groups for a subset of genes. A statistically significant different was also observed in percent cell death, cell cycle arrest and DNA repair between MPN and Control cell lines where LCLs from MPN patients exhibited high G Score value, showed resistance to cell death, bypassed cell cycle arrest and showed aberrant DNA repair. In addition a significant correlation was observed between most of the intermediate phenotypes and the combinations of multiple polymorphisms (G score). Thus these findings accentuate the importance of assessing a cumulative effect of panel of polymorphisms in modulating genotoxic sensitivity and emphasizes that factors such as extent of DNA repair, percent cell cycle delay might have potential significance in identifying susceptibility to UADT MPN. It also reinforces the assertion that identifying G score signature which can differentiate the study participants into two different subsets and its correlation with various phenotypic effects may have an important bearing on predisposing an individual to UADT MPN development.

Publications

1. Hussain T, Kotnis A, Sarin R and Mulherkar R. Establishment and characterization of lymphoblastoid cell lines from patients with Multiple Primary Neoplasms in the upper aero-digestive tract and healthy individuals. *Indian J Med Res.* 2012 Jun; 135(6):820-9.

2. Budrukkar A, Shahid T, Murthy V, Hussain T, Mulherkar R, Vundinti BR, Deshpande M, Sengar M, Laskar SG and Agarwal JP. Squamous cell carcinoma of base of tongue in a patient with Fanconi's anemia treated with radiation therapy: case report and review of literature. *Head & Neck,* 2010 Oct; 32(10):1422-7.

3. Hussain T and Mulherkar R. Lymphoblastoid cell lines: a continuous *in-vitro* source to study carcinogen sensitivity and DNA repair. (Review article; *International Journal of Cellular and Molecular Medicine*, in press).

4. Hussain T, Kotnis A, Sarin R and Mulherkar R. Genetic Susceptibility to Multiple Primary Neoplasms in the Upper Aero-Digestive Tract: Genotype Score and Phenotype Correlation. (communicated to *Cancer letters*)

Poster/oral presentations

1. International Society for Cell & Gene Therapy of Cancer (ISCGT) conference, India, 2007. (Participation)

2. 13th Human Genome Meeting "Genomics and the future of medicine", India, 2008.(Poster presentation)

3. 29th Annual Convention of Indian Association for Cancer Research, India, 2010.m(Oral presentation)

4. 6th Graduate Students Meet, ACTREC, Navi Mumbai, 2010. (Poster award)

5. 30th Annual Convention of Indian Association for Cancer Research and International Symposium on "Signalling Network and Cancer", CSIR-IICB, Kolkata, 2011. („Rajnikant Baxi‟ poster award)

6. 1st Global Cancer Genomics Consortium-Tata Memorial Centre, 2011. (Posteraward). American Association of Cancer Research (AACR) international conference on"New Horizons in Cancer Research: Biology to prevention to Therapy", 2011. (Poster presentation)

Name	:	**Yogendra Singh Rajpurohit**
Enrolment No.	:	LIFE01200704002
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Molecular Characterization of a Protein Kinase Involved in Extraordinary Radioresistance of Deinococcus Radiodurans

Abstract

Proteins are the ultimate biomolecules that determine the cellular functions in any living system. Adaptation of living organisms to different environmental conditions is regulated by differential activities of the proteins. Protein phosphorylation is an important modification that play role in regulation of protein functions and in conveying the impact of changes if any, to other molecules in the cellular *milieu* through signal transduction mechanisms. The involvement of protein phosphorylation in DNA damage response and cell cycle regulation is better understood in eukaryotes and the roles of Serine / Threonine protein kinase (STPK) in regulation of these processes have been reported. However, the involvement of protein phosphorylation and STPKs in bacterial response to radiation resistance and DNA damage is not well studied. The bacteria belongs to *Deinococcaceae* family are best characterized for their extraordinary tolerance to DNA damage. *Deinococcus radiodurans* R1 (DEIRA), a member of this family exhibits resistance to the lethal and mutagenic effects of various DNA damaging agents including radiations and desiccation. Unlike other bacteria, it lacks SOS response, characterized as a DNA damage response mechanism in bacteria. It therefore, offers, a potential model system for investigating the DNA damage response mechanism alternative to SOS response in this prokaryote. Initially it was observed that DEIRA genome annotates a pyrroloquinoline quinine (PQQ) synthase gene (pqqE), involves in PQQ biosynthesis in heterologous system and subsequently PQQ was shown to be an inducer of STPK in *E. coli*. The *pqqE* was deleted from genome of *D.* radiodurans and the mutant was found to be sensitive to gamma radiation. It showed a changed phosphoprotein profile and impaired DNA double strand break (DSB) repair as compared to wild type. The PQQ binding motifs search analysis in the DEIRA proteome showed that there were five hypothetical proteins encoded from *dr0503, dr0766, dr1769, dr2518 and drc0015* ORFs having multiple though, different numbers of PQQ binding motifs. These genes were individually deleted from genome of this bacterium and mutants were checked for gamma radiation survival. DR2518 deletion made significant impact and these cells were hypersensitive to gamma radiation and also to other DNA damaging agents. DR2518 was characterized as a radiation and PQQ, inducible eukaryotic type STPK having role in DNA damage tolerance and DSB repair of this bacterium. The Δdr2518 mutant showed a distinctly different phopshoprotein profile as compared to wild type. Lys42 amino acid of DR2518 was replaced with alanineand K42A mutant became inactive and it failed to complement the radiation resistance loss of *dr2518* mutant. The search for the presence of phosphoacceptor motif of eSTPKs in DEIRA proteome found many proteins containing the eSTPK phosphoacceptor motif. The phosphorylation of one of such protein, PprA (a pleotropic protein promoting DNA repair) by DR2518 resulted in the modulation of its known activities and failed to complement the radiation resistance loss of *pprA* mutant in *Deinococcus radiodurans.* The results presented in this thesis collectively suggest that DR2518, a eSTPK protein kinase plays important role in γ-radiation resistance and DSB repair of *D. radiodurans* perhaps through phosphorylation of DNA repair proteins. Results obtained from one such protein PprA phosphorylation by this kinase, on its both *in vitro* activity and *in vivo* functional complementation further supported the possibility of DNA repair functions modulation by phosphorylation.

Publications

1. Involvement of protein kinase activity inducer in DNA double strand break repair and radioresistance of *Deinococcus radiodurans*; Rajpurohit, Y. S., Gopalakrishnan R., and Misra H. S., *J. Bact*. 2008, 190: 3948-3954.

2. Characterization of a DNA damage inducible membrane protein kinase from *Deinococcus radiodurans* and its role in bacterial radioresistance and DNA strand break repair; Rajpurohit Y.S., Misra H.S.; Mol. Microbiol., 2010, 77 (6) : 1470-1482.

3. A eukaryotic type Ser/Thr protein kinase activity is required for its role in gamma radiation resistance and phosphorylation of DNA binding proteins in *Deinococcus radiodurans*. Yogendra S. Rajpurohit and Hari S. Misra (under revision at Journal of Biological Sciences)

BARC NEWSLETTER Reports

1. An antioxidant from a radioresistant bacterium: its role *in radiation resistance b*eyond oxidative stress tolerance. H.S. Misra, Y.S. Rajpurohit and N.P. Khairnar, BARC NEWSLETTER, p1-9 May-June 2010.

Papers presented during national symposia / seminars/ conferences

1. Rajpurohit Y.S., Misra H.S. A protein kinase activity inducer contributes to DNA double strand break repair and radioresistance in *Deinococcus radiodurans.* DAE-BRNS Life Science Symposium 2007 (LSS-2007), p-66, Dec.5-7, 2007, Mumbai.

2. Kamble V. A., Khairnar N. P., Rajpurohit, Y. S. and Misra H. S. Role of bacterial protein kinase autophosphorylation activity in DNA strand break repair. Proceedings of annual meetings of Indian Society of Cell Biologists, p-123, Dec. 14-16, 2007, Varanasi, India.

3. Rajpurohit Y. S. and Misra H. S. Involvement of a pyrroloquinoline –quinone binding protein kinase in DNA double strand break repair and radiation tolerance in *Deinococcus radiodurans.* Proceedings of international Conference on Radiation Biology, Abstract No. 159, Nov. 10-12, 2008, Jaipur, India.

4. Rajpurohit Y.S. and Misra H.S. PprA phosphorylation by STPK of Deinococcus radiodurans changes its in vitro functions. Poster presented at DAE-BRNS Life Science Symposium (LSS-2011), Anstract No. 12, p-54, Nov. 12-14, 2011, Mumbai, India.

Papers presented during international symposia / seminars/ conferences

1. Rajpurohit Y.S. and Misra H.S. Characterization of radiation inducible eukaryotic type serine / threonine protein kinase from *Deinococcus radiodurans.* 4th Congress of European Microbiologists, FEMS 2011, Abstract No. 258, p-144, June 26-30, 2011 Geneva, Switzerland.

2. Rajpurohit Y.S. and Misra H.S. DNA metabolic proteins phosphorylation by eukaryotic type Ser/Thr protein kinase impacts radiation resistance in *Deinococcus radiodurans* R1. 14th international workshop on ataxia-telangiectasia. P-97, February 7-11, 2012, New Delhi, India.

Gene Expression Omnibus submission:
GSM442568, GSE17722 (GSM442538, GSM442539, GSM442540, GSM442541)

Fellowship / Award/ other achievements

1. Received Travel grant from DST, for presenting my work entitled "Characterization of radiation inducible eukaryotic type serine / threonine protein kinase from *Deinococcus radiodurans"* authored as Rajpurohit Y.S. and Misra H.S. at 4th Congress of European Microbiologists, FEMS 2011, Geneva, Switzerland, June 26-30, 2011.

2. Received FEMS young scientist travel award for presenting my work "Characterization of radiation inducible eukaryotic type serine / threonine protein kinase from *Deinococcus radiodurans"* authored as Rajpurohit Y.S. and Misra H.S. at 4th Congress of European Microbiologists, FEMS 2011, Geneva, Switzerland, June 26-30, 2011.

3. Received Best poster award for presenting my work "PprA phosphorylation by STPK of *Deinococcus radiodurans* changes its *in vitro* functions*"* authored as Rajpurohit Y.S. and Misra H.S. at Life Sciences Symposium, 12-14 Nov 2011, Mumbai.

Name   :   **Sandeep Kumar Sharma**
Enrolment No.   :   CHEM01200804006
Constituent Institute   :   Bhabha Atomic Research Centre, Mumbai
Title   :   Study of Nanostructures using Positron Annihilation
                                Spectroscopy

Abstract

In the present work, positron and positronium have been used as probes for the investigation of molecular level vacant spaces (nanoholes) in polymers and atomic level defects in crystalline nanomaterials, respectively.

In literature, the triplet state of positronium (o-Ps) has been extensively used as probe to study the free volume in synthetic polymers. The o-Ps lifetime and corresponding intensity are related size and their density, respectively. However, use of o-Ps to study the nanostructure of natural polymers like starch as well as synthetic polymers modified by grafting, ion-irradiation and nanocompostite formatin is limited in literature. The study of nanostructure of these polymeric using o-Ps probe is expected to reveal new findings about the structure at manolevel. In the present thesis, nanostructure of starch/sucrose matrix has been studied as a function of temperature and absorbed water. It was observed that nanoholes size increases as a function of temperature. The nanohole density remain constant up to a certain temperature and further decreases in a two step function at higher temperature. Thus observed decrease is attributed to the decomposition of matrix to carbon black. In such a case, glass transition tempratiurre of the matrix was determined using a simple model which provides the nanoholes size in the absence of decomposition. With inclusion of water in the matrix, nanoholes size was observed to increase without any noticeable change in their density. It was observed that temperature and water have similar consequences of starch/sucrose matrix leading to glass transition process. Water molecules are uniformly distributed in the matrix through hydrogen bonding and do not block the existing nanoholes in the matrix.

Positron annihilation spectroscopy (PAS) supplemented with conventional measurement like Fourier Transform Infra Red (FTIR), Dynamic Mechanical Analysis (DMA) and X-ray Diffraction (XRD) has been used for the investigation of synthetic polymer based systems namely Acrylic acid grafted, CI ion-irradiated poly (ethylene terephthalate), PET, and phenolformaldehyde-carbon nanotube composites. The variations in o-Ps lifetime and intensity in PET grafted with acrylic acid were observed to follow the additive rule up to 6% followed by a complex behavior indicating the phase segregation

at higher degree of grafting. These observation were consistent with DMA results. On ion-irradiation of PET at lower fluence ($9x\ 10^9$ icons/cm^2 0, the changes were primarily see in nanohole size and concentration. No changes were obserced from FTIR and XRD data. The changes in nanoholes parameters were predominant at surface and subsurface region. Age Momentum Correlation measurements in phenolformadehyde resin-carbon nanotube composites showed o-Ps annihilation primarily occurs at the interfaces and a large fraction of free positrons annihilation in the carbon nanotubes dispersed in the polymer matrix. These observation were consistent with postitron lifetime measurements.

In recent years, PAS has been used for the investigation of electronic structure ofvarious nanoscale crystalline materials. In view of literature reports, itis found that positron systematics in nanoprticles is

not yet well understood and extensive studies are required. In the present study, positron lifetime and Coincidence Doppler broadening measurements have been carried out in semiconductor (ZnO and CdSe) and metal (Au) nanoparticles. These studies were corroborated with density function theory based calculation of positron parameters and formation and energy of vacancy defects. In case of ZnO, it was seen that ZnO, it was seen that Zn vacancies start migrating with increase in temperature and at very high temperature (800°C) they are annealed out. The concentration of Cd vacancies was observed to decrease in CdSe particle size. The present studies confirmed two types of vacancy defects, monovacancy and penta vacancy in square pyramidal configuration, as most probable defects in Au nanoparticles synthesized through chemical route.

Publications

Reffereed Journals

1. Positron annihilation studies in ZnO nanoparticles. S. K. Sharma, P. K. Pujari, K. Sudarshan, D. Dutta, M. Mahapatra, S.V. Godbole, O. D. Jayakumar and A. K. Tyagi *Sol. State Commun.* 149 (2009) 550.

2. Characterization of a sucrose/starch matrix through positron annihilation lifetimespectroscopy: unravelling the decomposition and glass transition processes.S. K. Sharma, G. Roudaut, I. Fabing and G. Duplâtre,*Phys. Chem. Chem. Phys.* 12 (2010) 14278.

3. Free volume and microstructural investigation of poly(ethylene terephthalate)-gacrylicacid(PET-g-AA) copolymer films.S. K. Rath, M. Patri, S. K. Sharma, K. Sudarshan and P. K. Pujari *Rad. Phys. Chem*. 79 (2010) 745.

4. Modification of microstructure of the surface and the bulk in ion-irradiated membrane studied using positron annihilation spectroscopy. S. K. Sharma, P. Maheshwari, D. Dutta, K. Sudarshan and P. K. Pujari *Rad. Phys. Chem.* 79 (2010) 1115 5.

5. Effect of water on glass transition in starch/sucrose matrices investigated through positron annihilation lifetime spectroscopy: a new approach. S. K. Sharma, A. Zaydouri, G. Roudaut and G. Duplâtre *Phys. Chem. Chem. Phys.* 13 (2011) 19338.

6. Direct evidence of Cd vacancies in CdSe nanoparticles: positron annihilation studies. S. K. Sharma, K. Sudarshan, P. Maheshwari, D. Dutta, P.K. Pujari*, C.P. Shah, M. Kumar, and P. Bajaj *Eur. Phys. J. B* 82 (2011) 335.

7. Effect of interfacial interaction on free volumes in phenol-formaldehyde resincarbon nanotube composites: Positron annihilation lifetime and age momentum correlation studies S. K. Sharma, J. Prakash, K. Sudarshan, P. Maheshwari, D. Sathiyamoorthy and P. K. Pujari *Phys. Chem. Chem. Phys.* 14 (2012) 10972.

8. Investigation of vacancy defects configurations in gold nanoparticles: Density Functional Theory (DFT) calculations and positron annihilation studies. S. K. Sharma, K. Sudarshan and P. K. Pujari (Manuscript under preparation)

Name	:	**Vishal Parashar**
Enrolment No.	:	LIFE01200604006
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	X-Ray Crystallographic Analysis of HIV-1 Protease Substrate/ Inhibitor Complexes

Abstract

Acquired Immunodeficiency Syndrome (AIDS) is the major pandemic of recent times and is caused by Human Immunodeficiency Virus (HIV) which, for its survival and infectivity depends on the catalytic activity of viral enzyme, HIV-1 protease. Therefore, inhibitors of HIV-1 protease are major drugs against AIDS. However, emergence of resistant mutations in HIV-1 protease under selection pressure limits the long term clinical efficacy of the drugs. There is thus a need for continuous improvement of existing drugs, and also for design of new HIV-1 protease inhibitors. Three dimensional structures revealing interactions of HIV-1 protease with inhibitors as well as with substrates/products would be key inputs in this process. The present thesis reports few such complex structures determined using the powerful method of X-ray crystallography. This thesis reports the first observation of catalytic water molecule (WAT1) along with the carboxy1 terminal product peptide generated in sity through cleavage of the full-length substrate bound in the active sites of the crystallized enzyme molecules. The structure is suggestive of the repositioning, during substrate binding, of the catalytic water for activation before nucleophilic attack. This structure further suggests that to achieve the goal of designing inhibitors very closely mimicking the transition- state, the hydrogen-bonding pattern between WAT1 and the enzyme should be replicated. Saquinavir (SQV) is the important protease inhibitor which Is currently used in the HIV-treatment-regimen. Mutations G48V and L90M in HIV-1 protease are major active site and non active site mutations producing resistance against SQV while C95F is the associated major non-polymorphic mutation. Three dimensional structures of G48V/C95F, L90M/C95F and C95F mutants of tethered HIV-1 protease complexed with the drug SQV, reported in this thesis, give insight into the mechanisms of drug resistance. Residues that are responsible for loss of van der Waals interactions between enzyme and inhibitor either directly because of conformational changes or indirectly because of reshaping of active site cavity have been identified. Although drug Nelfinavir (NFV) and SQV share common functional groups, D30N is a major mutation against the drug NFV, and does not provide resistance against the drug SQV. Structure of D30N mutant-SQV complex was solved and analysed to find reason for this phenomenon. Guidelines for chemical modifications of existing inhibitors for better performance have been suggested.

Publications

1. Vishal Prashar, Amit Das, Subhash Bihani, J.-L.Ferrer and M.V. Hosur (2009) Catalytic Water Co-Existing with a Product Peptide in the Active Site of HIV-1 Protease revealed by X-Ray Structure Analysis. PLoS ONE 4: e7860. doi:10.1371/journal.pone.0007860.

2. Vishal Prashar, Subhash C. Bihani, Amit Das, D.R. Rao and M.V. Hosur (2010) Insights into the mechanism of drug resistance: X-ray structure analysis of G48V/C95F tethered HIV-1 protease dimer/saquinavir complex. Biochem.Biophys. Res. Commun. 396: 1018–1023.

3. Vishal Prashar, Subhash Bihani, Amit Das, J.-L. Ferrer and M.V. Hosur (2011) Saquinavir resistance mechanism of non-active site mutants of HIV-1 protease. Acta Cryst A 67: C292-C293.

4. Vishal Prashar, Subhash Bihani, Amit Das, J.-L.Ferrer and M.V.Hosur; X-ray structure analysis of L90M/C95F and C95F mutants of tethered HIV-1 protease dimer in complex with saquinavir. (To be published)

5. Vishal Prashar, Subhash Bihani, Amit Das, J.-L.Ferrer and M.V. Hosur; X-ray structure analysis of D30N tethered HIV-1 protease dimer/saquinavir complex. (To be published)

Name	:	**Gagan Deep Gupta**
Enrolment No.	:	LIFE01200604008
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Structural and Functional Studies of Translin-Like Proteins

Abstract

Translin and translin associated factor-X (trax) proteins are very well conserved in higher eukaryotes. Both the proteins have together been involved in DNA recombination, mRNA regulation and transport, and siRNA processing. Translin alone forms a nucleicacid binding competent octameric complex and nucleic-acid binding domain results from a combination of basic motifs in octameric structure. Trax, however, forms a heteromeric complex with translin. We demonstrated that wild-type drosophila (*Drosophila melanogaster*) translin is DNA binding competent and forms an octamer like human translin. Three-dimensional structure of DNA-binding incompetent drosophila P168S mutant translin, elucidated with single crystal X-ray diffraction methods, revealed that it forms an open doughnut shaped tetramer. This altered quaternary structure resulted in abrogation of nucleic-acid binding ability of drosophila mutant translin. The analysis of all available translin structures suggested that up-down dimer is energetically stable and evolutionary conserved subunit in translin proteins. The critical role of C-terminal residues of translin protein in formation of oligomeric state, and hence in DNA binding activity, was confirmed by synthesis and characterization of a chimeric protein.

Another part of my research was aimed to characterize trax. A bacterial co-expression system was designed to purify human translin-trax complex as trax alone is not stable. Characterization of translin-trax complex, supported with bioinformatics analyses, established that trax adopts translin fold. The ssDNA-binding activity of trax was demonstrated for the first time using UV-crosslinking of radiolabled DNA. Novel DNAbinding motifs were also identified on trax sequence such that substitution in these dramatically reduced DNA binding activity of translin-trax complex. Further, an exhaustive database search led to discovery of a trax-like protein present in genomes of Chloroflexi and Archaea. Phylogenetic analysis revealed that prokaryotic trax is ancestor of eukaryotic translin and trax proteins, and translin evolved in eukaryotes after gene duplication. Taken together, the present thesis provides a critical structural insight into the molecular function of evolutionary related translin and trax proteins and their interaction with single-stranded nucleic acid.

Publications

Publications in international journals
The following manuscripts, relevant to work presented in the thesis, have been published /communicated.

1. Gupta GD, Makde RD, Rao BJ, Kumar V (2008) Crystal structures of drosophila mutant translin and characterization of translin variants reveal the structural plasticity of translin proteins. FEBS J 275:4235-49.

2. Gupta GD, Kumar V (2012) Identification of nucleic acid binding sites on Translinassociated factor X (TRAX) Protein. PLoS ONE 7:e33035.

3. Kumar V, Gupta GD (2012) Low-resolution structure of drosophila translin. FEBS Openbio 2:37-46.

4.   Gupta GD, Kale A, Kumar V (2012) Molecular evolution of translin superfamily proteins within the genomes of eubacteria, archaea and eukaryotes. Submitted. Entries of protein structures in the Protein Data Bank (PDB)

5.   Gupta GD, Makde RD, Kumar V (2007) Crystal structure of Drosophila melanogaster translin protein. PDB-ID 2QRX

6.   Gupta GD, Makde RD, Kumar V (2007) Crystal structure of Drosophila melanogaster translin protein. PDB-ID 2QVA.

7.   Kumar V, Gupta GD (2012) Crystal structure of Drosophila melanogaster translin protein. PDB-ID 4DG7.

Name	:	**Debes Ray**
Enrolment No.	:	PHYS01200704032
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Synthesis and Characterization of Block Copolymer-Mediated Gold Nanoparticles

Abstract

The field of nanoscience and nanotechnology deals with development and understanding of materials with at least one of its dimensions in nanoscale in the range 1-100 nm. Properties of these nanomaterials have been found to be significantly different from that of the compositional atoms as well as corresponding bulk materials. Nanoparticles, with all the three dimensions in nanoscale, represent the most widespread current form of nanomaterials and their striking features have been widely exploited for various multidisciplinary applications. Gold nanoparticles have recently become a fundamental building block in nanotechnology due to their unique optical, electronic, catalytic and chemical properties. They can be synthesized by different ways depending on their application requirements.

This thesis provides insight into the synthesis, characterization and applications of gold nanoparticles through a novel method using block copolymers. Use of block copolymers for the synthesis of gold nanoparticles has many advantages e.g. block copolymer not only plays the dual role of reductant and stabilizer but also provide an economical and environmentally benign way for the synthesis of gold nanoparticles at ambient conditions. We have looked into the understanding of tuning of different components and role of solution conditions for improvement of this block copolymer-mediated synthesis of gold nanoparticles. A multi-technique approach combing spectroscopy (UV-visible spectroscopy), microscopy (TEM) and scattering (DLS, SAXS and SANS) techniques has been used for the characterization of gold nanoparticles for obtaining complementary information for detailed studies of these systems.

The main findings of my research work are:

The optimization of block copolymer-to-gold salt for the synthesis of gold salt for the synthesis of gold nanoparticles has been identified and its mechanism has been understood. It is found that a minimum a minimum ratio of block copolymer-to-gold salt is required for maintaining the synthesis. The maximum yield by varying the gold salt or block copolymer concentration is limited by the aggregation of large sized nanoparticles formed at high block copolymer concentrations.

The role of self-assembly of block copolymer on the synthesis of gold nanoparticles has been established. The higher propensity of block copolymer to self-assemble enhances the formation of gold nanoparticles. For block copolymers to self-assemble or mediate in nanoparticle synthesis is driven by different forces.

Two novel method (step-addition method and additional reductant method) for stable high-yield synthesis of gold nanoparticles have been developed. These methods can enhance nanoparticle yield by manyfold than those earlier synthesis methods.

The interaction behavior of gold nanoparticles with two model proteins lysozyme and BSA has been examined and understood. The strong attractive electrostatic interaction between lysozyme with nanoparticle leads to phase separation whereas BSA adsorption through site-specific interaction on nanoparticle form stable nanoparticle-protein conjugates under physiological conditions.

Publications

In Refereed Journals

1. Step-addition method for enhancing the yield of gold nanoparticles in block copolymersolution D. Ray and V.K. Aswal J. Macromol. Sci. Part B: Phys. 49, 810-820 (2010).
2. Concentration Effect on Tuning of Block Copolymer-mediated Synthesis of Gol Nanoparticles D. Ray, V.K. Aswal and D. Srivastava J. Nanosci. Nanotechnol. 10, 6356-6362 (2010).
3. Correlating Self-Assembly of Block Copolymers for their Application in Synthesis of Gold Nanoparticles D. Ray, V.K. Aswal and D. Srivastava J. Nanosci. Nanotechnol. 11, 1905-1913 (2011).
4. Synthesis and Characterization of High Concentration Block Copolymer-mediated Gold Nanoparticles D. Ray, V.K. Aswal and J. Kohlbrecher Langmuir 27, 4048-4056 (2011).
5. Tuning of block copolymer-mediated synthesis of gold nanoparticles D. Ray, V.K. Aswal and D. Srivastava Int. J. Nanosci. 10, 1035-1038 (2011).
6. Multi-technique Approach for the Study of Block Copolymer-mediated Gold Nanoparticles D. Ray and V.K. Aswal Nanosci. Nanotechnol. Lett. 3, 603-611 (2011).
7. Optimization of Components in High-yield Synthesis of Block copolymer-mediated Gold Nanoparticles D. Ray and V.K. Aswal J. Nanopart. Res. 14, 778 (2012).
8. Probing Protein Adsorption on Gold Nanoparticles D. Ray and V.K. Aswal (Under preparation).
9. SANS Studies of Temperature-dependent Block Copolymer-mediated Synthesis of Gold Nanoparticles D. Ray, V.K. Aswal and J. Kohlbrecher (Under preparation).

In Conferences and Symposia:

1. SANS studies insight into improving of yield of block copolymer-stabilized gold nanoparticles D. Ray and V.K. Aswal AIP Conf. Proc. 1202, 219-224 (2009).
2. Room Temperature, High-yield Synthesis of Block Copolymer-mediated Gold Nanoparticles D. Ray, V.K. Aswal and J. Kohlbrecher AIP Conf. Proc. 1313, 192-194 (2010).
3. Block copolymer-mediated gold nanoparticles: Small-angle scattering studies D. Ray and V.K. Aswal Acta Cryst. A67, C401 (2011).
4. Combined Small-angle Neutron and X-ray Scattering Studies of Block Copolymer-mediated Gold Nanoparticles D. Ray and V.K. Aswal AIP Conf. Proc. 1349, 405-406 (2011).
5. Block Copolymer-dependence on High-Yield Synthesis of Gold Nanoparticles D. Ray, V.K. Aswal and J. Kohlbrecher AIP Conf. Proc. (in press).
6. Synthesis and characterization of block copolymer stabilized gold nanoparticles in aqueous solution at room temperature D. Ray and V.K. Aswal 20th Annual General Meeting of Materials Research Society of India, Saha Institute of Nuclear Physics, Kolkata, India (2009).
7. SANS study reveals for enhancing the yield of Gold Nanoparticles in Block Copolymer Solution D. Ray and V.K. Aswal Conference on Neutron Scattering and Mesoscopic Systems, International Centre/Goa University, Goa, India (2009).

8. SANS Study for Correlating Self–Assembly of Block Copolymers for their Application in Synthesis of Gold Nanoparticles L. Jyoti, D. Ray and V.K. Aswal Conference on Neutron Scattering and Mesoscopic Systems, International Centre/Goa University, Goa, India (2009).

9. Concentration Dependence Tuning of Block Copolymer-mediated Synthesis of Gold Nanoparticles D. Ray and V.K. Aswal Proceedings of DAE Solid State Physics Symposium 54, 303 (2009).

10. Effect of Variation of Chemical Structure of Block Copolymer on the Synthesis of Gold Nanoparticles L. Jyoti, D. Ray and V.K. Aswal Proceedings of DAE Solid State Physics Symposium 54, 285 (2009).

11. Synthesis and Characterization of Block Copolymer-mediated Gold Nanoparticles D. Ray, V.K. Aswal and D. Srivastava SERC School-cum-Conference on Rheology of Complex Fluids, IIT Madras, Chennai, India (2010).

12. Synthesis and Characterization of Block Copolymer-mediated Gold Nanoparticles D. Ray, V.K. Aswal and D. Srivastava International Conference on Advances in Electron Microscopy and Related Techniques, held at BARC, Mumbai, India (2010).

13. Synthesis and Characterization of High-Yield Gold Nanoparticles D. Ray and V.K. Aswal Mumbai-Pune Soft Matter Meeting, held at IIT Bombay, Mumbai, India (2010). 191

14. Multi-technique Approach for the Characterization of Block Copolymer-mediated Gold Nanoparticles D. Ray and V.K. Aswal 3rd International Symposium on Materials Chemistry, held at BARC, Mumbai, India (2010).

15. Multi-technique Approach for the Study of Block Copolymer-mediated Gold Nanoparticles D. Ray, V.K. Aswal, J. Kohlbrecher, E. Venugopal, G. Kumaraswamy and D. Srivastava Mumbai-Pune Soft Matter Meeting, held at TIFR, Mumbai, India (2011).

16. High Yield Synthesis of Gold Nanoparticles for their Interaction with Proteins D. Ray, S. Kumar and V.K. Aswal Mumbai-Pune Soft Matter Meeting, held at NCL, Pune, India (2011).

17. Stimuli-responsive tuning of Block Copolymer-mediated Gold Nanoparticles as characterized by SANS D. Ray and V.K. Aswal 1st Asia-Oceania Conference on Neutron Scattering, held at Tsukuba, Japan (2011).

18. Probing Protein Adsorption on Gold Nanoparticles D. Ray and V.K. Aswal International Conference on Nanoscience and Nanotechnology, held at Hyderabad, India (2012).

Name   : **Ashutosh Rath**
Enrolment No.   : PHYS07200604038
Constituent Institute   : Institute of Physics, Bhubenswar
Title   : Dynamic and Static TEM Studies on the Formation of Au-Si and
                               Au-Ge Nanostructures

Abstract

The thesis reports on the formation of Au-Si and Au-Ge nanostructures under different thermal annealing conditions achieved by varying parameters such as, pressure film thickness, substrate, presence or absence of native oxide on the substrate, temperature etc. The variation in the temperature dependent behavior of gold nanostructures on Si(100) surface in presence and absence of native oxide layer were studied in-situ using a hot stage holder in high vacuum(HV) condition (inside TEM). We showed that it is possible to grow well aligned symmetric (4-fold) gold silicide nano structures of different sizes on Si(100) Substrate by varying the temperature and interface conditions. Formation of oriented multifaceted gold nano/ microstructures has been investigated experimentally in Au films of various thickness (5.0, 11.7 and 50 nm) deposited on Si(100) surface, annealed at high temperature (~975° C) and low vacuum (~10^2 mbar) conditions. The role of native oxide layer on morphology, orientations of the structures was studied in detail. Interfacial oxide layer, low vacuum and high temperature annealing conditions are found to be necessary to grow multifaceted gold structures. Furthermore, the influence of vacuum conditions upon the formation of nanostructures in presence and absence of oxide layer has been reported by depositing ~2 nm Au on Si(100) using thermal evaporation method as well as MBE(molecular beam epitaxy) method followed by thermal annealing. For with oxide interface case, sample was annealed at high temperature (850°C) under both high vacuum (HV) and low vacuum (LV) conditions. In HV, gold silicide rectangles were observed following the four-fold symmetry of the substrate due to selective thermal decomposition of native oxide layer, where as in LV, it does not show any such formation. For MBE grown samples (without oxide case), Post annealing was done at 500°C in three different vacuum conditions: (1) low vacuum (LV) furnace (2) UHV (10^{-10} mbar) (MBE chamber), (3) HV chamber, Although well aligned nano rectangles were formed in both HV and LV cases, corner rounding is more prominent in LV case. In UHV case, random structures were formed having sharp corners. In all the above three cases, samples were exposed to air before annealing. In-situ annealing inside UHV chamber without exposing to air resulted in well aligned with sharp corners. The details about the role of surface oxide in the corner rounding process are discussed in this thesis.

In the second part of the thesis. The role of gold silicide nanostructures as as catalyast in the formation of lobe-lobe (bi-lobed) Au-Ge nanostructures under UHV conditions on clean Si(100) surfaces has been described. For this study, ~ 2.0 nm thick Au films were grown by MBE. Nearly square shaped gold silicide nano structures of average length ~ 48 nm were formed after UHV annealing at temperature ~500°C. Well ordered Au-Ge nanostructures where Au and Ge residing side by side (lobe-lobe structures) were formed. In our systematic studies, we demonstrated that, gold-silicide nano alloy formation at the substrate (Si) surface is necessary for forming phase separated Au-Ge bilobed nanostructures. To study this nano scale phase separation and its effect on the formation bilobed structures, the Si substrate is replaced by Ge(100) surface. For this study, a ~ 2.0 nm thick Au films were grown on Ge(100) substrate by MBE. Nearly square shaped Au$_x$Ge$_{1-x}$ nano structures were formed after UHV annealing at temperature ~500°C. A ~ 2 bm Ge film was further deposited on the annealed sample while the substrate was kept at 500°C. Well distributed Au-Ge nanostructures with Au on the top of the pedestal Ge were formed. It is very interesting to notice that no Au-Ge bilobed structures were formed. The

detail about the formation of Au-Ge nanostructures of different shaped has been discussed in this thesis. In this thesis work, characterizations have been performed using the Scanning transmission electron microscopy (STEM), TEM, Scanning electron microscope (SEM), Rutherford Backscattering Spectrometry (RBS), Energy dispersive spectroscopy (EDS), Electron energy loss spectroscopy (EELS) and Electron Backscatter Diffraction Technique (EBSD).

Publications

1. Epitaxial growth of Au-Ge nanostructures on Ge(100) surface under ultra high vacuum condition. A. Rath, J. K. dash, R. R. Juluri, A. Ghosh and P. V. Satyam, To be submitted (2012):arXiv:1208.0238

2. Dynamic and Static Transmission Electron Microscopy Studies on Structural Evaluation of Au nanoislands on Si (100) Surface. A. Rath, R. R. Juluri and P. V. Satyam *J. Crystal Growth* (Under review, 2012): arXiv:1204.4618.

3. Structural Modi¯cation in Au/Si(100) system: Role of surface oxide and vacuum level. A. Rath, J. K Dash, R. R. Juluri and P. V. Satyam, *J. Vac. sci. technol. A-Lett.*(Under review, 2012): arXiv:1204.5370

4. Nano scale phase separation in Au-Ge system on ultra clean Si(100) surfaces. A. Rath, J. K. Dash, R. R. Juluri, Marco Schoewalter, Knut Mueller, A. Rosenauer and P.V. Satyam, *J. Appl. Phys.* 111, 104319 (2012): arXiv:1202.0614.

5. Growth of Oriented Au Nanostructures: Role of Oxide at the Interface. A. Rath, J. K. Dash, R. R. Juluri, A. Rosenauer, Marco Schoewalter and P.V. Satyam, *J. Appl. Phys.* 111, 064322 (2012):arXiv:1203.0819

6. Temperature dependent electron microscopy study of Au thin ¯lms on Si(100) with and without native oxide layer as barrier at the interface. A. Rath, J. K. Dash, R. R. Juluri, A. Rosenauer and P.V. Satyam, *J. Physics D: Applied Physics* 44, 115301 (2011).

7. Shape Evolution of MBE grown Si 1¡x Ge*x* Structures on High Index Si(5 5 12) surfaces : A temperature tempendent study J. K. Dash, A. Rath, R. R. Juluri and P. V.Satyam, *J. Physics D: Applied Physics* (In press, 2012): arXiv:1205.6039

8. Universality in Shape Evolution of Si 1¡x Ge*x* Structures on High Index Silicon Surfaces J. K. Dash, T. Bagarti, A. Rath, R. R. Juluri and P. V.Satyam, *Euro. Phys. Lett.* (In press, 2012): arXiv:1204.0578

9. Migration and extrusion of metal nanowire inside the ¯lled multi-walled carbon nanotube Pawan K. Tyagi,Umananda M Bhatta, Ashutosh Rath, J. Raghavendra Rao,Jatis K. Dash,Sanjeev Kumar, and P V Satyam, *Carbon*(Under review, 2012)

10. MeV Au2+ ions induced surface patterning in silica P. Santhana Raman, K.G.M. Nair, M. Kamruddin, A.K. Tyagi, A. Rath, P.V. Satyam, B.K. Panigrahi and V. Ravichandran. *Applied Surface Science* 258, 4156-4160(2012)

11. Epitaxy-like orientation of nano scale Ag islands grown on air-oxidized Si(110)- (5£1) surfaces. Anupam Roy, J. K. Dash, A. Rath and B. N. Dev, Accepted in *Surface and Interface Anlysis(2011)(wileyonlinelibrary.com) DOI 10.1002/sia.3837*.

12. Synthesis of re-dispersible Ce3+ co-doped LaPO4:Tb3+ nanorods and effcts of concentrations of Ce3+ or Tb3+ and reaction medium on luminescence properties: luminescence switching behavior through redox reaction and polymer films. G. Phaomei,R. S. Ningthoujam,W.R.Singh, R.S. Loitongbam,N.S.Singh, Ashutosh Rath, R. R. Juluri and R. K. Vatsa, *Dalton Trans.* 40, 115301(2011).

13. Shape transformation of Si1¡x Ge*x* structures on ultra clean Si (5 5 7) and Si (5 5 12) surfaces. J. K. Dash, A.Rath, R. R. Juluri,P Santhana Raman, K. Muller,M. Schowalter, R.Imlau, A. Rosenauer and P.V. Satyam *J. Phys.: Conf. Ser.* 326, 012021(2011).

14. DC heating induced shape transformation of Ge structures on ultra clean Si (5 5 12) surfaces J. K. Dash, A. Rath, R. R. Juluri,P Santhana Raman, K. Muller, A. Rosenauer and P.V. Satyam , *J. Phys.: Condens. Matter* 23, 135002 (2011).

15. Oxidation of Ion Beam Synthesized Embedded indium Nanoclusters in Silica. P. Santhana Raman, K.G.M. Nair, Ashutosh Rath, P.V. Satyam, B.K. Pani- grahi and V. Ravichandran, *Eur. Phys. J.:Applied Physics* 53, 30403 (2011).

16. Growth of SnO2/WO3- nano wire hierarchical hetero-structure and their appli- cation as chemical sensor. S. Sen, P. Kanitkar,A.Sharma, K. P. Muthe, Ashutosh Rath, S. K.Deshpande, M. Kaur,R. C. Aiyer, S. K. Gupta and J. V. Yakhmi *Sensors and Actuators B: Chemical*, 147, 453-460(2010).

17. Antiferro to superparamagnetic transition on Mn doping in NiO, P. Mallick, Chandana Rath, A. Rath, A. Banerjee and N. C. Mishra, *Solid State Communications,* 150, 1342-1345(2010).

18. Real-time study of oxide mediated liquid-solid growth of high aspect ratio aligned gold silicide microrods on Si(110) substrates. Umananda M. Bhatta, Ashutosh Rath, Jatis K. Dash, Jay Ghatak, Lai Yi-Feng, Chuan-Pu Liu and P. V. Satyam, *Nanotechnology* 20, 465601 (2009).

19. Structural phase transitions in Au thin ¯lms on Si (110): An *in-situ* temperature dependent transmission electron microscopy study. Umananda M. Bhatta, J. K. Dash, A. Rath and P. V. Satyam, *Appl. Surf. Sci.* 256, 567 (2009).

20. Formation of aligned nano-silicide structures in MBE grown Au/Si(110) system: A real-time temperature dependent TEM study. Umananda M. Bhatta, J. K. Dash, Anupam Roy, A. Rath and P. V. Satyam, *Phys: Cond. Matt.* 21, 205403 (2009).

21. Surface and Interfacial Structural Characterization of MBE Grown Si/Ge Multilayers. Biswajit Saha, Manjula Sharma, Abhisakh Sarma, Ashutosh Rath, P.V. Satyam, Purushottam Chakraborty, Milan K. Sanyal, *Applied Surface Science,* 256, 547-551(2009).

Conference Presentations

1. Shape transition in Au/Si(100) System : Role of surface oxide and vacuum Level. A. Rath, J. K. Dash, R. R. Juluri and P. V. Satyam, *ICONSAT-2012*, Hyderabad, India.

2. Shape transition in Au/Si(100) hetero epitaxial system: Role of vacuum level during annealing Ashutosh Rath, J. K. Dash, R. R. Juluri and P. V. Satyam, *ICANN-2011*, Guwahati,Assam, India.

3. Nano pattern formation in Ge/Au/Si(100) hetero epitaxial system A. Rath, J. K. Dash, R. R. Juluri and P.V. Satyam, *IINM-2011,*International conference on Ion beam induced nano patterning of materials Institute of Physics, Bhubaneswar,India.

4. Temperature dependent structural phase transformation from nano to microstruc- tures: A real time TEM study. Umananda M. Bhatta, J. Ghatak, A. Rath, J. K. Dash, P. Santhana Raman and P. V. Satyam, *PSI - 2009*, International Conference on Physics at surfaces and interfaces, Puri,India.

5. Formation of AuSi microrods on Si(110) surface: A real time TEM study. Umananda M. Bhatta, J. Ghatak, A. Rath, P. Santhana Raman, P.V.Satyam, *DAE-Solid State Physics Symposium* (India) 53,809(2008).

Name   :   **Raktim Dasgupta**
Enrolment No.   :   PHYS03200704006
Constituent Institute   :   Raja Ramanna Centre for Atomic Research, Indore
Title   :   Optical Micromanipulation Techniques and their Applications

Publications

1.   R. Dasgupta, R. S. Verma, S. Ahlawat, A. Uppal, and P. K. Gupta. "Studies onerythrocytes in malaria infected blood sample with Raman optical tweezers," *J. Biomed. Opt.* **16**, 077009 (2011). Also selected for the July 15, 2011 issue of Virtual Journal of Biological Physics Research.

2.   R. Dasgupta, S. Ahlawat, R. S. Verma, and P. K. Gupta, "Optical orientation and rotation of trapped RBCs with Laguerre-Gaussian mode," *Opt. Exp.* **19**, 7680-7688 (2011). Also selected for the July 1, 2011 issue of Virtual Journal of Biomedical Optics.

3.   R. Dasgupta, R. S. Verma, S. Ahlawat, D. Chaturvedi, and P. K. Gupta, "Long distance axial trapping with Laguerre-Gaussian beams," *Appl. Opt.* **50**, 1469-1476 (2011)Alsoelected for the July 1, 2011 issue of Virtual Journal of Biomedical Opt

4.   R. Dasgupta, S. Ahlawat, R. S. Verma, S. Shukla, and P. K. Gupta. "Optical trapping of spermatozoa using Laguerre-Gaussian laser modes," *J. Biomed. Opt.* **15**, 065010 (2010). Also selected for the July 1, 2011 issue of Virtual Journal of Biological Physics Research.

5.   R. Dasgupta, S. Ahlawat, R. S. Verma, A. Uppal, and P. K. Gupta. "Hemoglobindegradation in human erythrocytes with long duration near infrared laser exposure in Raman optical tweezers," *J. Biomed. Opt.* **15**, 055009 (2010). Also selected for the October 15, 2011 issue of Virtual Journal of Biological Physics Research.

6.   S. Ahlawat, R. Dasgupta, and P. K. Gupta, "Optical trapping near a colloidal cluster formed by a weakly focused laser beam," *J. Phys. D: Appl. Phys.* **41,** 105107 (2008).

7.   R. Dasgupta, S. Ahlawat, and P. K. Gupta, "Trapping of micron sized objects near a free liquid surface," *J. Opt. A: Pure Appl. Opt.* **9,** S189-S195 (2007).

In Edited Volumes :

1.   P.K.Gupta., S.K.Majumder and R.Dasgupta "Raman spectroscopy for biomedical diagnosis," AIP Conference Proceeding 1267, 135-136 (2010).

2.   S.Alhawat, R.Dasgupta and P.K.Gupta, "Optical trapping near a charged surface: three-dimensional optical binding of colloids," Proceedings of SPIE 6535, 65350W (2007).

In Conferences/Sympoai:

1.   P.K.Gupta, k. Divakar Rao, S.K.Majumder and R Dasgupta, "Optical Imaging and Diagnosis-some Recent Developments at RRCAT," December 2010 issue of Kiran-A Bulletin of Indian Laser Association, Natioanal Laser Symposium (NLS-19), Indore, India, 1-4 December, 2010.

2.   P.K.Gupta., S.K.Majumder and R.Dasgupta "Raman spectroscopy for biomedical diagnosis," XXII International Conference on Raman Spectroscopy (ICORS-2010), Boston, USA, 9-13 August, 2010.

3. R.Dasgupta, S.Ahlawat, R.S.Verma, S. Shukla and P.K.Gupta, "Laguerre Gaussian laser trapping of sperm cells with minimized photodamage," Photonics-2010, International conference on fiber optics and photonics, Guwahati, India, 11-15 December, 2010.

4. R.Dasgupta and P.K.Gupta "Raman spectroscopic studies of optically trapped red blood cells," Topical Conference on Interaction of EM Radiation with Atoms, Molecules and Clusters (TC-2010), Indore, India, 3-6 March, 2010. .

5. R.Dasgupta, R.S.Verma, S.Ahlawat, A.Uppal and P.K.Gupta, "Raman spectroscopic studies on optically trapped red blood cells in malaria infected blood sample,"International Conferemce on Laser Applications in Life Sciences, Oulu, Finland, 9-11 June, 2010.

6. R.Dasgupta, SAhlawat, R.S.Verma, A.Uppal and P.K.Gupta, "Raman spectroscopic study of hemoglobin degradation in optically trapped erythrocytes," XII International Conference on Laser Applications in Life Sciences, Oulu, Oulu, Finland, 9-11 June, 2010.

7. R.Dasgupta, R.S.Verma, S.Ahlawat, A.Uppal and P.K.Gupta,"Study on Red Blood Cells in Mararia infected Blood Sample with Raman Optical Tweezers," Indo-French workshop on Biomedical Applications of Vibration Spectroscopy and Imaging, Mumbai, India, 13-15 February, 2010.

8. R.Dasgupta, S.Ahlawat and P.K.Gupta, "Trapping of micron sized objects near a free liquid surface," Photonics-2006 (eighth international conference on optoelectronis, fiber optics and photonis), Hyderabad, India, 13-16 December, 2006.

Other Publications related to the thesis work:

1. R.Dasgupta and P.K.Gupta, Optical Tweezers and Cytometry, Chapter 13 in Advanced Optical Flow Cytometry : Methods and Disease Diagnoses Ed. By V.V.Tuchin, Wiley VCH, 2011. Pp363-386.

2. T.Gigrs, R.Dasgupta and P.K.Gupta, "Axial displacement Measurement of A Trapped Object using Principal components Analysis," Photonis-2008, International conference on fiber optics and photonics, New Delhi, India 13-17 December, 2008.

Name	:	**Dayamoy Banerjee**
Enrolment No.	:	CHEM01200604035
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Physiconchemical studies on the recovery and immobilization \ of radiocesium

Abstract

^{137}Cs, an important fission product, has immense potential as gamma source in radiation technology applications. The use of ^{137}Cs in place of ^{60}Co is advantageous particularly from source replacement point of view. In fact, ^{137}Cs is the ideal isotope for use in gamma chambers (GCs) and blood irradiators (BIs) where source requirement is not very high. Traditionally, ^{137}Cs in the form of CsCl powder encapsulated in double wall stainless steel capsules has been used as source. However, because of safety concerns, the ^{137}Cs in an immobilized form with suitable product characteristics is desirable.

With this objective, work pursued addresses some important aspects on recovery of ^{137}Cs for nuclear waste and immobilization of the radioelement in borosilicate matrix. Studies on the separation and recovery of ^{137}Cs from acidic as well as alkaline waste streams have been carried out employing Ammonium Molybdophosphate (AMP) coated on PMMA beads and resorcinol formaldehyde polycondensate resin, respectively. Extensive characterizations of the sorbents and correlation of the batch results with column performance have been carried out. Results of these studies are useful in formulating a comprehensive scheme for the recovery of purified ^{137}Cs product from HLW/ILW.

The letter part of the study concentrated on the development of suitable glass formulation for immobilization of the recovered Cs solution. Owing to the higher loading of alkali oxides including Cs_2O in glass, preparation of the glasses with higher chemical durability and minimum volatilization loss of Cs are the major challenges in the work. A large number of glasses of verying compositions have been prepared and characterized. Detailed investigations on the durability and Cs volatilization behavior have been carried out. Efforts were also made to evaluate the structural changes brought out by the incorporation of the different additives. The structural information obtained was used to explain the observed properties of the glasses. Results of volatilization study confirmed that volatilization of Cs from all the glasses followed a diffusion controlled process. A structural model has been proposed and used to explain the observed variation in the activation energies and frequency factor for Cs diffusion. Based on these screening studies, three glass formulations have been

shortlisted. Long duration leaching studies and measurement of the extent of Cs volatilization have been carried out with the shortlisted formulations. Result of the study is useful in selection of glass formulations for use as radiation source in blood irradiators.

Publications

Journal

1. D. Banerjee, M.A. Rao, J. Gabriel and S.K. Samanta, _Recovery of Purified Radiocesium from Acidic Solution using Ammonium Molybdophosphate and Resorcinol Formaldehyde Polycondensate Resin', Desalination 232, 172-180, 2008.

2. D. Banerjee, V. Sudarsan, A. Joseph, R.K. Mishra I.J. Singh, P.K. Wattal and D. Das, _Role of TiO2 on Physico-Chemical Properties of Cesium Borosilicate Glasses', J. Am. Ceram. Soc. 93 [10] 3252–3258, 2010.

3. D. Banerjee, V. Sudarsan, A. Joseph, I.J. Singh, J. Nuwad, C.G.S. Pillai, P.K. Wattal and D. Das, Physicochemical properties of Cs borosilicate glasses containing CaO, J. Nucl. Mater. 413, 177–182, 2011.

4. D. Banerjee, A. Joseph, V. Sudarsan, P.K. Wattal and D. Das, Effect of composition and temperature on volatilization of Cs from borosilicate glasses, J. Am. Ceram. Soc. (95 [4] 1284–1289 (2012).

5. D. Banerjee, M. A. Rao and P.K. Wattal, Separation and recovery of Cs from high active waste simulant using resorcinol formaldehyde polycondensate resin: Batch and column studies, Sep. Sci.Technol. (Accepted).

6. D. Banerjee, V. Sudarsan, P.K. Wattal and D. Das, Role of structural groups on chemical durability of high Cs bearing sodium borosilicate glasses containing CaO, Phys. Chem. Glasses. (accepted).

7. D. Banerjee, V. Sudarsan, A. Joseph, P.K. Wattal and D. Das, Evaluation of the suitable divalent cations for the preparation of Cs-borosilicate glasses for use as a gamma source, Phys. Chem. Glasses. (communicated).

8. D. Banerjee, Annie Joseph, V. Sudarsan, P.K. Wattal and D. Das, 137Cs based borosilicate glass source for radiation technology applications. Glass Technology, (communicated).

Conferences

1. D. Banerjee, Annie Joseph, I.J. Singh, P.K. Wattal and D.Das, _Development of 137Cs based borosilicate glass source in radiation technology applications', NUCAR-2011, Visakhapatnam, Feb-22-26, 2011.

2. R.K. Gupta, Sugilal Gopalakrishnan, S.B Patil, Piyush Srivastava, Jyoti Jha, K.N.S. Nair, D. Banerjee, —Wealth from Waste – Demonstration of Selective Removal of

3. Cesium from Radioactive Wastes for Producing Blood Irradiator Source Pencils', - 11626, WM Symposia, USA, Jan-2011

4. D. Banerjee, A. Joseph, I.J. Singh and P.K. Wattal, _Effect of Bivalent Cations on the Physicochemical Properties of Cs-Borosilicate Glasses', Proc. ISMC-2010. Mumbai, Dec7-11, 2010.

5. D. Banerjee, I.J. Singh, P.K. Wattal, _Evaluation of Cs-borosilicate glass formulation on the basis of mixed alkali effect for use as a source in radiation technology applications', Proc. of International Workshop & Symposium on Synthesis and Characterization of Glass/Glass-ceramics (IWSSCGGC-2010), Pune, India, July 7-10, 2010.

6. Amar Kumar, P.S. Dhami, Tessy Vincent, S.B. Patil and D. Banerjee, _Recovery of Valuable Fission Products from Radioactive Waste', Proc. *Peaceful Uses of Atomic Energy – 2009, New Delhi, Oct 1-3, 2009*

7. D. Banerjee, M.A. Rao and S.K. Samanta, _Column Loading and Elution Behavior of Rubidium during Ion Exchange Separation of Cesium from Alkaline Radioactive Waste', Proc. of DAE-BRNS Symp. on Emerging Trends in Sep. Sci. Technol. SESTEC – 2008, University of Delhi, Delhi, March 12-14, 2008, page -173.

8. D. Banerjee, M.A. Rao, J. Gabriel and S.K. Samanta, _Evaluation of some Process Variables for the Separation of 137Cs from Acidic Solution using Ammonium Molybdophosphate', Proceedings of DAE-BRNS Symposium on Emerging Trends in Separation Science and Technology, SESTEC – 2006, Mumbai, Sept. 29-Oct. 1, 2006, page -260.

9. D. Banerjee, M.A. Rao and S.K. Samanta, _Ion Exchange Purification of 137Cs after Caustic Dissolution of 137Cs-loaded Ammonium Molybdophosphate', Proceedings of DAE-BRNS Symposium on Emerging Trends in Separation Science and Technology, SESTEC – 2006, Mumbai, Sept. 29-Oct. 1, 2006, page -262.

Name	:	**Shekar Goud**
Enrolment No.	:	PHYS06200704002
Constituent Institute	:	Institute for Plasma Research, Gandhinagar
Title	:	Optical Micromanipulation Techniques and their Applications

Abstract

In a simple toroidal plasma, it is well known that single particle confinement and hence the equilibrium does not exist. The observed plasma confinement time in the experiments is, however, found to be at least an order higher than that is theoretically predicted using single particle and ExB drifts. It is understood, therefore, that there must be some mechanism similar to rotational transform in tokamaks. In the present work, the role of fluctuations and intrinsic poloidal flows in sustaining mean profiles has been experimentally investigated in a simple magnetized toroidal plasma device (BETA).

To begin with, the existence of large fluctuations and filling of plasma in the entire radial domain are observed to be associated with each other. Simultaneous measurements on high field side (HFS) and low field side (LFS) have indicated that the onset of fluctuations on LFS is followed by density build-up on HFS. In order to understand this correlation more quantitatively, various poloidal flow velocity is of the order of mean electric field driven flow under some conditions. Interestingly, the fluctuation induced flow is opposite in direction to the mean electric field driven flow, partially accounting for the observed difference between the net flow and the mean electric field driven flow. On increasing the toroidal magnetic field strength, a transition occurs in the nature of fluctuations, from highly coherent at low magnetic field to turbulent at high magnetic field, accompanied by the enhanced poloidal flow and increased densities on HFS. Similar studies have been performed with increasing ion mass. The present work demonstrates that in a toroidal compressible plasma, a strong correlation exists between fluctuations, intrinsically generated poloidal flows and enhanced densities.

Publications

1. Experimental determination of radial spread of residual fast electrons in a hot _lament toroidal magnetized plasma, T. S. Goud, R. Ganesh, K. Sathyanarayana,

2. D. Raju, K. K. Mohandas, C. Chavda, A. M. Thakar and N. C. Patel, J. of Phys.: Conf. Ser. 208, 012029 (2010).

3. Role of fluctuations and flows in sustaining mean proifiles in a current less toroidal plasma_, T. S. Goud, R. Ganesh, Y. C. Saxena, D. Raju, K. Sathya- narayana, K. K. Mohandas and C. Chavda, Phys. Plasmas 18, 042310 (2011).

4. Coherent to turbulence transition, enhanced flow and confinement in a simple toroidal plasma, T. S. Goud, R. Ganesh, Y. C. Saxena, D. Raju, K. Sathyanarayana, K. K. Mohandas and C. Chavda, Phys. Plasmas 19, 032307 (2012).

5. Role of ion mass in fluctuations and poloidal flows in a simple toroidal plasma, T. S. Goud, R. Ganesh, Y. C. Saxena and D. Raju, Phys. Plasmas 19, 072306 (2012).

6. Statistical properties of _uctuation induced poloidal flux and flow in a current less toroidal plasma_, T. S. Goud, R. Ganesh, D. Raju and Y. C. Saxena, manuscript under preparation

Name   :   **Siddhartha Mukhopadhyay**
Enrolment No.   :   ENGG01200704024
Constituent Institute   :   Bhabha Atomic Research Centre, Mumbai
Title   :   Identification of Dynamic System in the Presence of Noise with
                                 Wavelets as Basis Functions

Abstract

The work in the thesis addresses the problem of identification of complex systems in presence of noise. Modeling complexities with wavelet basis improves prediction capability and robustness of identified model. A novel technique for estimating parameters of a strictly time varying model in wavelet domain is proposed based on consistent output prediction as an alternative solution to the classical least squares minimization problem. The work introduces and justifies the use of spline biorthogonal wavelets as a modeling tool for system identification. It suggests that weighted scalar summation of projections in approximation space could be used for deriving consistent output prediction in case model structure is built with spline biorthogonal wavelets. The method of identification could be viewed as modeling with pre-filtered input and output which renders the identified model minimum-memory (ideal case) and insensitive to noise. Resulting parameter estimates are unbiased and bounded.

An iterative algorithm, alternately projecting the solution in time and wavelet domain for penalized minimization of local error in wavelet coefficients, is proposed for output reconstruction. The algorithm is computationally efficient and exhibits excellent performance in cross validation. Stability and uniqueness issues of reconstruction by alternate projection is studied. As an extension of existing methods of reconstruction from sparse wavelet representation, a new representation called wavelet maximum curvature point representation is proposed. The algorithm ensures that the reconstructed signal contains complete information for characterization. The technique is validated by characterizing NDT signals.

As a case study, the paper addresses the problem of modeling a complex process called the Liquid Zone Control System (LZCS) in a large Pressurized Heavy Water Reactor based on the evolution of input and output. In this work, an identification scheme of a linear time invariant model of the LZCS is studied. Orthogonal as well as biorthogonal wavelets are used for consistent output estimate of the LZCS process. The technique is verified on the real experimental data obtained from a full scale test setup.

The concept of designing an admissible control, constrained to be memory-less, with output wavelet states is introduced and controllability of the open loop and closed loop system with output feedback is studied. The theory of controller design with wavelet states is developed in the work. The technique is demonstrated with simulation examples of multi-scale systems. Point kinetic model of a nuclear reactor is studied for pole assignment by designing a wavelet state controller.

Publications

1. S. Mukhopadhyay, U. Mahapatra, A. K. Tangirala and A. P. Tiwari, Spline wavelets for system identification, Proceedings of DYCOPS 2010, Leuven, Belgium, 2010.

2. S. Mukhopadhyay and A. P. Tiwari, Characterization of NDT signals: Reconstruction from wavelet transfor maximum curvature representation, Signal Processing, 90(1), 261-268, 2010.

3. S. Mukhopadhyay and A. P. Tiwari, Consistent output estimate with wavelets: An alternative solution of least squares minimization problem for identification of the LZC system of a large PHWR, Annals of Nuclear Engineering, 37(7), 974-984, 2010.

Name	:	**Santosh Kumar Das**
Enrolment No.	:	PHYS04200704002
Constituent Institute	:	Variable Energy Cyclotron Centre, Kolkatai
Title	:	Heavy Flavor Production and Propagation in Heavy Ion Collision

Abstract

The Theory of strong interaction – Quantum Chromodynamics (QCD) has a unique feature _ it possess the properties of asymptotic freedom which implies that at very high temperatures and/or densities nuclear matter will exist in a deconfined state of quarks and gluons _ called Quark Gluon Plasma (QGP). Recent lattice QCD based calculations confirm that the typical value of temperature for the quark_hadron transaction is O(150-180) MeV. It is expected that QGP can be created in the laboratory by colliding nuclei at relativistic energies. The relativistic Heavy Ion Collider (RHIC) Brookhaven and the Hadron Collider (LHC) at CERN, Geneva are two experimental facilities where matter in the state of QGP can be created. In QGP some of the symmetries of the physical vacuum may either be restored or broken - albeit transiently.

In these contexts, the study QGP becomes a field of high contemporary interest and the heavy flavors namely, charm and bottom quarks play a crucial role in such studies, because they are produced in the early stage of the collisions and they do not dictate the bulk properties of the matter. Therefore, the propagation of heavy quarks through QGP may be treated as the interactions between equilibrium and non-equilibrium degrees of freedom. Fokker-Planck (FP) equation provides an appropriate framework for such studies. In this work the FP equation has been used to study the propagation of charm and bottom quarks hot and dense QGP.

The drag and diffusion coefficients of charm and bottom quarks have been evaluated for both collisional and radiative processes using pQCD techniques. The dead cone and Landau-Pomeronchuk-Migdal (LPM) effects on the radiative loss of heavy quarks have been considered. Bothe radiative and collisional processes of energy loss are included in the effective drag and diffusion coefficients. For the initial distribution, we have employed the c-quark spectra produced in p-p collisions. With the effective transport coefficients and the initial distribution, the FP equation has been solved for the the heavy qurks executing Brownian motion in the the QGP. The solution of the FP equation have been convoluted with the relevant fragmentation functions to obtain the D and B meson spectra. The $_{PT}$ distribution of electrons originating from the decays of the D and B mesons have been calculated.

The solution of the FP equation has been used to evaluate the nuclear suppressions factor, R_{AA} and the elliptic flow, $_{U2}$ for the non-photonic single electron spectra resulting from the semi-leptonic decays of hadrons containing charm and bottom quarks. The effect on non-zero baryonic chemical potential on the drag and diffusion coefficients of heavy quarks propagating through a baryon rich quark gluon plasma have been studied.

Whether QGP is produced or not the formation of hadronic system is inevitable in high energy heavy ion collision. Therefore, dissipation of heavy flavored meson in hadronic medium assumes importance. In this context the drag and diffusion coefficients of the hadronic matter have been evaluated and its implication to heavy ion collision have been discussed in this dissertation.

Publications

1. Probing Quark Gluon Plasma Properties by Heavy Hlavors. Santosh K Das, Jane Alam and Payal Mohanty Phys. Rev C 80, 054916(2009) arXiv:0910.4856.

2. Nuclear Suppression at Low Energy in Relativistic Heavy Ion Collision. Santosh K Das, Jane Alam, Payal Mohanty and Bikash Sinha Phys. Rev C 81, 044912(2010) arXiv:0910.4853

3. Dragging Heavy Quarks in Quark Gluon Plasma at the Large Hadron Collider. Santosh K Das, Jane Alam and Payal Mohanty Phys. Rev C 82, 014908(2010) arXiv:1003.5508

4. Soft Gluon Multiplicity Distribution Revisited. Santosh K Das and Jane AlamPhys Rev D 82 (Rapid), 051502(R) (2010) arXiv:1007.4405

5. Transport Coefficients of Gluonic Fluid. Santosh K Das and Jane Alam Phys Rev D 83, 114011(2011) arXiv: 1011.4181

6. Dragging D Mesons by Hot Hadrons. Sabyasachi Ghosh, Santosh K Das, Sourav Sarkar and Jane Alam Phys Rev D 84 (Rapid), 011503(R) (2011) arXiv: 1104.0163

7. Momentum Dependence of Drag Coefficients and Heavy Flavour Dup-pression in Quark Gluon Plasma. Surasree Majumdar,Trambak Bhattacharyya, Jane Alam and Santosh K Das Phys Rev C 84, 044901(2011) arXiv:1106.2615

8. Energy Loss of Fast Gluons in a Gluonic Fluid. Trambak Bhattacharyya, Surasree Majumdar, Santosh K Das and Jane Alam Phys Rev D 85, 034033(2012) arXiv:1106.0609

9. Radial Flow From Electromagnetic Probes and Signals of Quark Gluon Plasma. Payal Mohanty, Jajati K Nayak, Jane Alam and Santosh K Das Phys Rev C 82, 034901(2010) arXiv:0910.4856

10. Elliptic Flow of Thermal Dileptons as a Probe of QCD Matter. Payal Mohanty, Victor Roy, Sabyasachi Ghosh, Santosh K Das, Bedangadas Mohanty, Sourav Sarkar, Jane Alam and Asis K Chaudhuri Accepted for publication in Phy. Rev. C (Rapid) arXiv:1111.2159

Conference Proceeding in Journal

1. Heavy Flavour Suppression and Flow. Santosh K Das and Jane Alam Nucl. Phys. A, 862-863 (2011) 289-292 arXiv:1101.3385

2. Probing Quark Gluon Plasma by Heavy Flavors. Santosh K Das and Jane Alam. To be published in POS, WPCF,2012 arXiv:1202.1428

3. Equilibration in Quark Gluon Plasma. Santosh K Das, Jane Alam, and Payal Mohanty Indian J.Phys.85:1149-1153,2011 arXiv:0912.4089

Arxiv Submission

1. Elliptic Flow of Heavy Flavors.Santosh K Das and Jane Alam arXiv:1008.2643

2. Transport Coefficients of B Mesons in Hot Hadronic Matter. Santosh K Das, Sabyasachi Ghosh, Sourav Sarkar and Jane Alam arXiv:1109.3359

Conference Proceeding

1. Heavy Flavour Production and Propagation in Heavy Ion Collisions. Santosh K Das Proc. of DAE Symp. on Nucl. Phys. (India) 56 (2011) 1178

2. Transport Coefficients of B Mesons in Hot Hadronic Matter. Santosh K Das, Sabyasachi Ghosh, Sourav Sarkar, Jan-e Alam Proc. of DAE Symp. on Nucl. Phys. (India) 56 (2011) 944

3. Dragging D by Hot Hadrons. Sabyasachi Ghosh, Santosh K Das, Sourav Sarkar, Jan-e Alam Proc. of DAE Symp. on Nucl. Phys. (India) 56 (2011) 974

4. Shear Viscosity of a Pion Gas. Sukanya Mitra, Santosh K Das, Sourav Sarkar, Jan-e Alam Proc. of DAE Symp. on Nucl. Phys. (India) 56 (2011) 978

5. On the Soft Gluon Radiation in Partonic Plasma. Trambak Bhattacharyya, Surasree Mazumder, Santosh K Das, Jan-e Alam Proc. of DAE Symp. on Nucl. Phys. (India) 56 (2011) 904.

6. Charged Hadron Hroduction in Proton-Proton Collisions at LHC Energy. Santosh K Das, Nihar R Sahoo, Sudipan De and Tapan Nayak Proc. of DAE Symp. on Nucl. Phys. (India) 56 (2011) 988

7. Probing Elliptic Flow of QCD Matter by Lepton Pairs. Payal Mohanty, Victor Roy, Sabyasachi Ghosh, Santosh K Das, Bedangadas Mohanty, Sourav Sarkar, Jan-e Alam, Asis K Chaudhuri Proc. of DAE Symp. on Nucl. Phys. (India) 56 (2011) 910

8. Heavy Flavours as a Probe of Quark Gluon Plasma. Santosh K Das and Jane Alam Proc. of DAE Symp. on Nucl. Phys. (India) 55 (2010) 584.

9. Flow From Electromagnetic Radiation. P. Mohanty, J. K. Nayak, Jan-e Alam and Santosh K Das Proc. of DAE Symp. on Nucl. Phys. (India) 55 (2010) 628

10. Radiative Energy Loss in Gluon Gas. Santosh K Das and Jan-e Alam Proc. of DAE Symp. on Nucl. Phys. (India) 55 (2010) 626.

11. Freeze Out Time in Ultra-Relativistic Heavy Ion Collisions. Santosh K Das, Payal Mohanty, Jajati K Nayak and Jan-e Alam Proc. of DAE Symp. on Nucl. Phys. (India) 52 (2007) 521

Name	:	**Rana Nandi**
Enrolment No.	:	PHYS05200704006
Constituent Institute	:	Saha Institute of Nuclear Physics, Kolkata
Title	:	Studies on Some Aspects of Neutron Stars- From Crust to Core

Abstract

In this thesis we have studied the ground state composition of crustal matters of ordinary neutron stars as well as magnetars. For the outer crust, the most recent experimental mass table has been used to get the nuclear energy. Strong magnetic fields are found to enhance the electron number density appreciably . This helps some new and heavier nuclei to appear in the sequence of nuclei of the outer crust. Also, the neutron drip density is found to be shifted to higher densities.

Ground state properties of the inner crust has been investigated in the Thomas-Fermi model and using the separation procedure of Bonche, Levin and Vautherin to extract the nuclei from the background of neutron gas. Like the outer crust here also strong magnetic fields cause the electron density to increase which in turn enhances the proton fraction. As a result, less number of neutrons drip out of the nuclei and the equilibrium nuclei become heavier. Strong magnetic fields also reduce the free energy to make the system more bound, compared to the field free scenario. We also calculate the shear mode frequencies for magnetars by taking the effect of magnetic fields on the composition of the crust and reproduce most of the observed quasi-periodic oscillation frequencies of soft gamma-ray repeaters.

We also calculate the shear viscosity of neutron star core in presence of an antikaon condensate. It is found that the onset of kaon condensation causes a steep drop in the electron and the muon shear viscosities. The appearance of kaon condensate also enhances the proton fraction appreciably and it makes the proton shear viscosity to be comparable to that of neutron's at higher densities. We also calculate the neutrino shear viscosity in neutrino-trapped matter of proto-neutron stars and study its role on the thermal nucleation rate of the antikaon condensed phase. It is observed that the influence of shear viscosity on the thermal nucleation time is significant.

Publications

1. Neutron Star Crust in Strong Magnetic Fields R Nandi and D Bandyopadhyay *J. Phys. Conf. Ser.* 312 042016 (2011).

2. Inner crust of neutron stars in strongly quantizing magnetic fields R Nandi, D Bandyopadhyay, I N Mishustin and W Greiner *Astrophys. J.* 736 156 (2011).

3. Shear viscosity in antikaon condensed matter R Nandi, S Banik and D Bandyopadhyay *Phys. Rev. D* 80 123015 (2009).

4. Nucleation of antikaon condensed matter in protoneutron stars S Banik and R Nandi *AIP Conf. Proc.* 1441 396 (2011).

5. Shear viscosity and the nucleation of antikaon condensed matter in protoneutron stars S Banik, R Nandi and D Bandyopadhyay *Phys. Rev. C* 84 065804 (2011).

6. Melting of antikaon condensate in protoneutron starsS Banik, R Nandi and D Bandyopadhyay, *arXiv:*astro-ph/1206.1701.

7. Role of strongly magnetized crusts in torsional shear modes of magnetars R Nandi, D Chatterjee and D Bandyopadhyay, *arXiv:*astro-ph/1207.3247.

Name   :   **Pankaj Kandwal**
Enrolment No.   :   CHEM01200704002
Constituent Institute   :   Bhabha Atomic Research Centre, Mumbai
Title   :   Studies on the Separtion of Cesium and Strontium from Acidic
                                  Solutions using Liquid Membranes

Abstract

The thesis gives a detailed account of the use of solvent extraction and supported liquid membrane transport behavior of Cs(I) and Sr(II) using macrocyclic extractants. CNC (calix[4]arene-bis-2,3-naphtho-crown-6) has been used as a selective extractant for cesium which shows 1000 times better selectivity for Cs as compared to other alkali metal ions such as Na, K etc. On the other hand, di-*tert*-butylcyclohexano 18-crown-6 (DtBuCH18C6) has been successfully employed as selective carrier ligand for strontium. The recovery of Cs and Sr from PHWR-SHLW feed solution has been successfully demonstrated on 0.5 L scale by HFSLM technique. A mathematical model has also been developed for the mass transfer modeling of the transport process of metal ion through the membranes. The recycling of the organic solvent has been carried out to ensure the long term application in the reprocessing of radioactive waste.

A HFSLM method has also been developed for the carrier free separation of 90Y from ^{90}Sr-^{90}Y. In an approach for simultaneous recovery of Cs and Sr, a new solvent system (NPOE + *n*-dodecane) has been developed for CCD and PEG-400 and is successfully demonstrated by solvent extraction studies. Although these studies have shown quite interesting results, yet the membrane transport experiments were negative. However, Cs(I) transport data were encouraging. The thesis work has resulted in 6 research papers in peer reviewed International journals and 12 symposia papers.

Publications

1. Selective cesium transport using hollow fibre supported liquid membrane containing calix[4]arene-bis-napthocrown-6 as the carrier extractant. P. Kandwal, P.K. Mohapatra, S.A. Ansari and V.K. Manchanda, *Radiochim. Acta*, 98 (2010) 493-498.

2. Separation of carrier free 90Y from 90Sr by hollow fiber supported liquid membrane containing bis(2-ethylhexyl) phosphonic acid. P. Kandwal, S.A. Ansari, P.K. Mohapatra and V.K. Manchanda, *Sep. Sci. Technol.,* 46(6), (2011) 904-911.

3. Mathematical modeling of Cs(I) transport through flat sheet supported liquid membrane using calix-[4]-bis(2,3-naptho)-18-crown-6 as the mobile carrier. P. Kandwal, S. Dixit, S. Mukhopadhyay, P.K. Mohapatra, V.K. Manchanda, *Desalination,* 278 (2011) 405-411.

4. Mass transport modeling of Cs(I) through hollow fiber supported liquid membrane containing calix-[4]-bis(2,3-naptho)-crown-6 as the mobile carrier. P. Kandwal, S. Dixit, S. Mukhopadhyay, and P.K. Mohapatra, *Chemical Engineering Journal,* 174 (2011) 110– 116.

5. Transport of cesium using hollow fiber supported liquid membrane containing calix[4]arene-bis(2,3-naphtho)crown-6 as the carrier extractant: Part II. Recovery from simulated high level waste and mass transfer modeling. P. Kandwal, S.A. Ansari and P.K. Mohapatra, *J. Membr. Sci.,* 384 (2011) 37-43.

6. A Highly Efficient Supported Liquid Membrane System for Near Quantitative Recovery of ` Radio-strontium from Acidic Feeds: Part II. Scale up and Mass Transfer Modeling in Hollow Fiber Configuration. P. Kandwal, S.A. Ansari and P.K. Mohapatra, *J. Membr. Sci.,* 405-406, (2012) 85- 91.

7. Selective Recovery of Am(III) over Eu(III) by Hollow Fiber Supported Liquid Membrane Using Cyanex 301 in the Presence of Synergists as the Carrier. A. Bhattacharyya, S. A. Ansari, P. Kandwal, P. K. Mohapatra, and V. K. Manchanda, *Sep. Sci. Technol.,* 46 (2011) 205–214.

8. A 'cold' actinide partitioning run at 20 L scale with hollow fibre supported liquid membrane using diglycolamide extractants. S. A. Ansari, R. B. Gujar, P. K. Mohapatra, P. Kandwal, A. Sengupta, S. K. Thulasidas and V. K. Manchanda, *Radiochim. Acta,* 99 (2011) 815-821.

9. Pertraction of plutonium in the +4 oxidation state through a supported liquid membrane containing TODGA as the carrier. S. Panja, P.K. Mohapatra, P. Kandwal, S.C. Tripathi, V.K. Manchanda, *Desalination,* 262 (2010) 57-63.

10. Evaluation of polymer inclusion membranes containing calix[4]-bis-2,3-napthocrown- 6 for Cs recovery from acidic feeds: Transport behavior, morphology and modeling studies. D.R. Raut, P. Kandwal, G. Rebello, P.K. Mohapatra, J. Membr.   Sci., 407– 408 (2012) 17– 26.

Name	:	**Anil Jain**
Enrolment No.	:	PHYS01200804021
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Investigation of Structural and Magnetic Properties of Spin-Chain Oxides

Abstract

In the present thesis work, structural and magnetic properties of the geometrically frustrated spin-chain compound $Ca_3Co_2O_6$, $Ca_3Co_{2-x}Fe_xO_6$, and $Ca_{2.75}R_{0.25}Co_2O_6$ (R = Lu and Dy) have been investigated using x-ray and neutron powder diffraction, dc magnetization, and Mössbauer spectroscopy techniques. All compounds (except Ca_3CoFeO_6) crystallize in the space group R $\overline{3}$ c. For the compounds $Ca_{2.75}R_{0.25}Co_2O_6$ (R = Lu and Dy), a reduction in the oxidation state of the cobalt ions at the trigonal prism site (6a) has been observed with R substitution. For all compounds (except Ca_3CoFeO_6), the magnetic structure, below T_N, corresponds to an incommensurate spin density wave structure, having a modulation and an alignment of the spins along the crystallographic c axis., which is quite different from the reported partially disordered antiferromagnetic (PDA) structure for these compounds. Further, a coexistence of the magnetic long-range and short-range ordering has been observed (below T_N). For the parent compound $Ca_3Co_2O_6$, in addition to the magnetic Bragg peaks corresponding to the SDW structure, a second set of magnetic peaks corresponding to the commensurate antiferromagnetic (CAFM) structure are observed below ~ 15 K. Besides, a strong time dependence of the intensities of both CAFM and SDW structures has been observed at 10 K. For the Fe-substituted compounds $Ca_3Co_{2-x}Fe_xO_6$ (x ≤ 0.4), a decrease in the intrachain positive exchange constant (J) and an increase in the interchain negative exchange constant (J') have been observed with increasing the concentration of Fe, which result in deviation from "1D character" in these spin-chain compounds. Field induced magnetic phase transitions have also been observed in the neutron diffraction as well as dc magnetization study.

Publications

1. Short-range and long-range incommensurate magnetic ordering in the frustrated antiferromagnets $Ca_3Co_{2-x}Fe_xO_6$: A neutron diffraction study A. Jain and S.M. Yusuf Phys. Rev. B 83, 184425 (2011).

2. Magnetic ordering in the spin-chain compounds $Ca_3Co_{2-x}Fe_xO_6$ (*x* = 0.2 and 0.4): A neutron diffraction study A. Jain, S. M. Yusuf, J. Campo, and L. Keller Phys. Rev. B 79, 184428(2009).

3. Effect of Fe substitution on the magnetic ordering in $Ca_3(Co_{1-x}Fe_x)_2O_6$ I. Nowik, A. Jain, S. M. Yusuf, and J. V. Yakhmi Phys. Rev. B 77, 054403 (2008).

4. Neutron diffraction study of quasi-one dimension spin chain compounds $Ca_3Co_{2-x}Fe_xO_6$ A. Jain, S. M. Yusuf, and Sher Singh Pramana – J. Phys. 71, 923 (2008). Structural and Magnetic properties of the layered compound $Ca_{2.375}La_{0.125}Sr_{0.5}GaMn_2O_8$ A.K. Bera, S. M. Yusuf, and A. Jain Pramana – J. Phys. 71, 917 (2008).

5. Structural and Magnetic Properties of Spin Chain Compounds $Ca_3Co_{2-x}Fe_xO_6$ A. Jain, Sher Singh, and S. M. Yusuf Phys. Rev. B 74, 174419 (2006). Field-induced incommensurate-to-commensurate magnetic phase transition in $Ca_3Co_{1.8}Fe_{0.2}O_6$: A neutron diffraction study S. M. Yusuf, A. Jain, and L. Keller, Phys. Rev. B (under review).

Name	:	**Madhumita Halder**
Enrolment No.	:	PHYS01200604001
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Structral and Magnetic Properties of Magnetocaloric Materials

Abstract

The main objective of the present thesis is investigation of structural and magnetic properties as well as the nature of magnetic phase transition of various intermetallic compounds showing large magnetocaloric effect (MCE). When an external magnetic field is applied to a magnetic material, there is a change in the magnetic entropy of the material. This change in magnetic entropy on application of magnetic field is termed as MCE. The nature and order of magnetic phase transitions play vital roles in determining the magnitude of the magnetic entropy change, and its dependence on temperature and magnetic field. To tune the properties of a magnetic material suitable for magnetic refrigeration, it is important to understand its structural and magnetic properties.

A wide class of intermetallic compounds with diversity in their nature of magnetic ordering and phase transition, such as compounds with ferromagnetic ordering, mixed ferromagnetic and antiferromagnetic ordering, metamagnetic transition, magnetostructural transition *etc.* has been investigated. A detailed study has been carried out on tailoring the magnetic properties including phase transitions of these intermetallic compounds. The importance of exchange interaction and universality class in determining MCE has been brought out in this thesis by investigating the intermetallic compound $TbCo_{2-x}Fe_x$ and $Mn_4FeGe_{3-x}Si_x$. The critical exponent study near the Curie temperature for $TbCo_2$ and $TbCo_{1.9}Fe_{0.1}$ compounds was carried out to analyze the nature of the magnetic phase transition. The derived values of critical exponents represent the phenomenological universal curve for the field dependence of magnetic entropy change curve. For the $Mn_4FeGe_{3-x}Si_x$ compounds, the author has also used such a phenomenological curve for these compounds to deduce the critical exponents. Thus, studying MCE for a particular material is not only important for its practical application point of view but it also provides a tool to understand the properties of the material. In particular, the details of the magnetic phase transition and critical behavior of a given material can be obtained by studying the MCE of the material. The transition from antiferromagnetic to ferromagnetic state in semi-Heusler alloys $Cu_{1-x}Ni_xMnSb$, has been investigated in details in the region x < 0.3. In the region, $0.05 \leq x \geq 0.2$, it has been observed that with decrease in temperature, there is a transition from paramagnetic to ferromagnetic state, and below ~ 50 K both antiferromagnetic and ferromagnetic phase coexist. The importance of phase coexistence in obtaining a broad operating temperature range for MCE has been brought out in case of $Cu_{1-x}Ni_xMnSb$ semi-Heusler alloys. The importance of interesting phenomena such as metamagnetic transitions and domain wall pinning in obtaining large MCE and an inverse MCE, respectively, has been brought out in intermetallic compounds $NdMn_{2-x}Co_xCo_xSi_2$.

Publications

Journals

1. Magnetic properties and magnetocaloric effect in intermetallics compounds $NdMn_2-xCoxSi_2$. S. M. Yusuf, M. Halder, A. K. Rajarajan, A. K. Nigam, and S. Banerjee J. Appl. Phys. 111, 093914 (2012).

2. Enhancement of ferromagnetism in Ni excess $Cu_{1-x}Ni_xMnSb$ half Heusler alloys. B. L. Ahuja, A. Dashora, S. Tiwari, H. S. Mund, M. Halder, S. M. Yusuf, M. Itou, and Y. Sakurai J. Appl. Phys. 111, 033914 (2012).

3. Magnetocaloric effect and its implementation in critical behavior study of $Mn_4FeGe_{3-x}Si_x$ intermetallic compounds. M. Halder, S. M. Yusuf, and A. K. Nigam J. Appl. Phys. 110, 113915 (2011).

4. Investigation of magnetic phase transition in $TbCo_{2-x}Fe_x$. M. Halder and S. M. Yusuf BARC Newsletter, Founder's Day Special Issue, 290 (October 2011).

5. Crossover from antiferromagnetic to ferromagnetic ordering in semi-Heusler alloys $Cu_{1-x}NixMnSb$ with increasing Ni concentration. M. Halder, S. M. Yusuf, A. Kumar, A. K. Nigam, and L. Keller Phys. Rev. B 84, 094435 (2011).

6. Magnetocaloric effect and critical behavior near the paramagnetic to ferromagnetic phase transition temperature in $TbCo_{2-x}Fe_x$. M. Halder, S. M. Yusuf, M. D. Mukadam, and K. Shashikala Phys. Rev. B 81, 174402 (2010).

Papers published/presented in conferences/symposia

1. Crossover from antiferromagnetic to ferromagnetic state in the semi Heusler alloys $Cu_{1-x}Ni_xMnSb$ M. Halder and S. M. Yusuf AIP Conf. Proceedings 1447, 1179 (2012).

2. Appearance of ferromagnetism in the antiferromagnetic CuMnSb on Ni substitution. M. Halder, S. M. Yusuf, and A. K. Nigam AIP Conf. Proceedings 1349, 1193 (2011).

3. Second order magnetic phase transition in $TbCo_{2-x}Fe_x$. M. Halder and S. M. Yusuf AIP Conf. Proceedings 1347, 67 (2011).

4. Transition from antiferromagnetic to ferromagnetic State in $Cu_{1-x}Ni_xMnSb$. M. Halder, S. M. Yusuf, and A. K. Nigam 3*rd* DAE-BRNS International Symposium on Materials Chemistry (2010).

5. A Crossover from short-range to long-range exchange interaction in $TbCo_{2-x}Fe_x$. M. Halder and S. M. Yusu Conference on Advance in Magnetism: Phenomena and Materials (2010).

6. Magnetostructural phase transition in $TbCo_{2-x}Fe_x$: A neutron diffraction study. M. Halder, S. M. Yusuf, and K. Shashikala Solid State Physics 54,173 (2009).

7. Magnetostructural phase transition in $TbCo_{2-x}Fe_x$: A neutron diffraction study. M. Halder, S. M. Yusuf, and K. Shashikala Conference on Neutron Scattering and Mesoscopic Systems (2009) .

8. Magnetocaloric effect in $TbCo_{1.94}Fe_{0.06}$. M. Halder, S. M. Yusuf, and K. Shashikala Solid State Physics 53,1193 (2008).

9. Hydrogen absorption studies on $Tb(Co_{0.95}Fe_{0.05})_2$. K. Shashikala, M. Halder, S. M. Yusuf, and C. G. S. Pillai Solid State Physics 53,1281 (2008).

10. Study of magnetocaloric effect in $TbCo_{1.9}Fe_{0.1}$. M. Halder, S. M. Yusuf, and K. Shashikala 2*nd* DAE-BRNS International Symposium on Materials Chemistry (2008) .

11. Influence of Fe substitution on the magnetocaloric effect in $TbCo_2$. M. Halder, S. M. Yusuf, and K. Shashikala International Conference on Magnetic Materials and their Application for 21st Century (2008).

Name	:	**S. Anand**
Enrolment No.	:	PHYS01200704019
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Study of Coagulation of Dispersing Aerosol Systems

Abstract

The present thesis deals with study of coagulation of dispersing aerosol systems. A key question for assessing the impact of anthropogenic and natural aerosols on the environment pertains to the estimation of the fraction of particles from various sources that persist in the atmosphere to form background aerosols. The present study addresses this question by combining the coagulation with dispersion for different emission scenarios to understand the long time and far-field behaviour of aerosol number concentration and size spectra.

Comprehensive numerical and analytical models are developed to obtain solutions to the coagulation-dispersion equation for the puff, plume, and continuous volumetric releases. The combined action of coagulation and dispersion reduces the total particle number concentration significantly in a high concentrated release of aerosol particles near the source. The fraction of particles surviving the coagulation in the puff or plume is termed as 'survival fraction' or 'source term modifier'. The two specific objectives met in this study are, 1) obtaining simpler expressions or approximations for the survival fraction for puff and plume releases, and 2) estimation of important metrics like total number concentration, average particle size, etc., in the case of continuous volumetric releases.

The study brings out several important features of the coagulation-dispersion process affecting the evolution of particles released into environment. These include the effects of mode of release and the various aerosol and environmental parameters on particle number concentrations and effective sizes. Furthermore, this thesis brought out the relevance of this study to estimate aerosol number loading factors in the context of air pollution studies.

Publications

1. S. Anand, Y.S.Mayya, Coagulation in a diffusing Gaussian aerosol puff: Comparison of analytical approximations with numerical solutions, *Journal of Aerosol Science*, 40 (2009) 348-361.

2. S. Anand, Y.S.Mayya, A simplified approach for solving coagulation-diffusion equation to estimate atmospheric background particle number loading factors contributed by emissions from localized sources, *Atmospheric Environment*, 45 (26) (2011) 4488-4496.

3. S. Anand, Y.S. Mayya, M. Yu, M. Seipenbusch, G. Kasper, A numerical study of coagulation of nanoparticle aerosols injected continuously into a large, well stirred chamber, *Journal of Aerosol Science*, 52 (2012) 18-32.*

Presentations in Conferences and Workshops attended

1. S. Anand, Y.S.Mayya, A study on simultaneous coagulation and dispersion in a concentrated aerosol cloud, *Indian Aerosol Science and Technology Association (IASTA-2007) Conference on Emerging Trends in Aerosol Technology and Applications*, Nov 14-16, 2007 at NPL, New Delhi.

2. S. Anand, Y.S.Mayya, Modeling source strength modification due to coagulation in a diffusing aerosol puff, *European Aerosol Conference (EAC-2009)*, Sep 6-11, 2009 at University of Karlsruhe, Karlsruhe, Germany. * Contributions – S.A., and Y.S.M. designed the study and developed the models. M.Y., M.S., and G.K. provided the experimental parameters for model comparisons.

Name	:	**Subhash Chandra Bihani**
Enrolment No.	:	LIFE01200604004
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Understanding Drug Resistance in HIV-1 Protease through X-ray Crystallography

Abstract

Acquired Immuno Deficiency Syndrome (AIDS) caused by Human Immunodeficiency Virus (HIV) is a major epidemic of the modern world, and HIV-1 protease inhibitors are major class of drugs used for the treatment of HIV-AIDS. An atomic level understanding of the mechanisms of catalysis and drug resistance in HIV-1 protease are needed to overcome drug-resistant virus. This thesis reports sample preparation and X-ray crystallographic results obtained in an effort to throw light on these mechanisms. The first part of the thesis describes the structure of a complex between proline containing oligo-peptide substrate and an active HIV-1 protease enzyme. Being the first such structure to be reported, it suggests a different mechanism for hydrolysis of an internal peptide bond next to a proline residue. The second part of the thesis describes crystal structures of unliganded and nelfinavir-bound HIV-1 protease harboring nelfinavir resistance mutations D30N, L90M, N88D, and N88S. In case of D30N mutation, a crucial hydrogen bond between the drug and the 30th residue is weakend in the mutant. In N88S mutant, a large conformational change in residue D30, very likely, eliminates the hydrogen bond with the drug. In N88D the active site volume is increased resulting in sub-optimal binding of the drug nelfinavir. In drug-resistant HIV, the mutations D30N and L90M in the protease enzyme are never observed together, and the crystal structures suggest that the catalytic activity of this double mutant may be reduced to a level that would make survival and replication of the mutant virus Impossible. The Structure of N88S enables, through molecular modeling, retionalization of hypersusceptibility of N88S against amprenavir.

Publlications

1. Bihani S C, Das A, Prashar V, Ferrer J-L and Hosur M V (2009) Resistance mechanism revealed by crystal structures of unliganded nelfinavir-resistant HIV-1 protease non-active site mutants N88D and N88S. Biochem Biophys Res Comm 389: 295–300.

2. Bihani S C, Das A, Prashar V, Ferrer J-L and Hosur M V (2008) X-ray structures of HIV-1 protease-in-situ product complex. Proteins: Struct Func Bioinfo, 74: 594-602.

3. Hosur M V, Prashar V, Das A, and Bihani S (2008) Structural investigations of HIV-1 protease complex with substrates and inhibitors; In 37th National Seminar on Crystallography at Kolkata (India), IT4.

4. Bihani S C, Ferrer J-L and Hosur M V. Molecular basis for mutual exclusivity of D30N and L90M in HIV-1 protease. Manuscript under preparation.

5. Bihani S C, Ferrer J-L and Hosur M V. Effect of drug resistance mutation D30N on the binding of drug nelfinavir. Manuscript under preparation.

Name	:	**Prasana Kumar Sahoo**
Enrolment No.	:	PHYS02200704020
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	Quasi One Dimensional GaN Nanostructures: Growth Kinetics, Physical Properties, and Applications

Publications

1. Prasana Sahoo, S. Dhara, S. Amirthapandian, M. Kamruddin, S. Dash, A. K. Tyagi, *Role of surface polarity in self-catalyzed nucleation and evolution of GaN nanostructures,* Crystal Growth & Design, 2012, 12, 2375-2381

2. Prasana Sahoo, S. Dhara, S. Dash, I. Manna, B. Raj, A. K. Tyagi, *"Air trapped nano-cavity induced superhydrophobicity on GaN microbelt"* Appl. Phys. Lett. 2011, 98, 043103-043105. [Featured in *Nature India highlight* "Water repelling surface sensor" and Virtual J. of Nanoscale Science & Technology, Vol. 23, Issue 5 (2011)]

3. Prasana Sahoo, D. S. Oliveira, M. A. Cotta, S. Dhara, S. Dash, A. K. Tyagi, B. Raj, *"Enhanced surface potential variation on nanoprotrusions of GaN microbelt as a probe for humidity sensing"* J. Phys. Chem. C, 2011, 115, 5863-5867.

4. Prasana Sahoo, J. Basu, S. Dhara, H. C. Fang, C. P. Lu, T. R. Ravindran, S. Dash and A. K. Tyagi, *"Single step growth dynamics and multi-functional properties of core-shell GaN on Ga2O3 freestanding microbelts",* J. Mater. Sci., 2012, 47, 3447-.3453

5. Prasana Sahoo, S. Dhara, S. Dash, A. K. Tyagi, *GaN Nanostructures: Growth Kinetics and Applications,* Nanoscience & Nanotechnology-ASIA, 2011, 1, 140–161 (Invited Review)

6. Prasana Sahoo, S. Dhara, C. R. Das, S. Dash, A. K. Tyagi, B. Raj, P. Chandramohan, M. P. Srinivasan*, "Surface optical modes in GaN nanowires"* Int. J. Nanotech., 2010, 7, 823-832.

7. Prasana Sahoo, Avinash Patsha, S. Dhara, S. Dash, M. Kamruddin, R. Pandian, A. K. Tyagi, *Scaling of beaded GaN with pressure in self-catalyzed anisotropic growth technique,* Int. J. Material Physics, 2012 (In Press; not included in thesis)

Submitted for review

8. Prasana Sahoo, S. Sumathi, S. Dhara, G. Saini, S. Rangarajan, S. Dash, A. K. Tyagi, *Directlabel Free Ultrasensitive Impedimetric Genosensor using Dendrimer Functionalized GaN Nanowires,* Analytical Chemistry, 2012 (Under Review)

9. Prasana Sahoo, P. S. Murthy, S. Dhara, V. P. Venugopala, A. Das, A. K. Tyagi, *Probing the Dynamics of Cellular Damage and protein expression in Bacterial Cells Induced by GaN Nanoparticles using Confocal Laser Raman spectroscopy,* J. Phys. Chem. C, 2012 (Under Review)

10. Prasana Sahoo*,* S. Dhara, S. Dash, S. Amirthapandian, A. K. Prasad, A. K. Tyagi, *Room temperature H2 sensing using Pt- functionalized GaN nanotubes,* J. Phys. Chem. C, 2012 (Under Review)

11. Prasana Sahoo, S. Dhara, S. Dash, A. K. Tyagi, *Photo-assisted local oxidation, and fragmentation by ultra small Pt nanoclusters functionalized single GaN Nanotubes,* J. Nanopart. Res. 2012 (Under Review)

Book Chapter

12. S. Dhara, Prasana Sahoo, A. K. Tyagi, B. Raj *"Surface Optical Modes in Semiconductor Nanowires,* Nanowires - Implementations and Applications, Intech- Open Access Book, pp- 1-26, ISBN 978-953-307-318-7; http://www.intechopen.com/books/nanowires-implementations-and-applications/surface-optical-modes-in-semiconductor-nanowires

Manuscript under Preparation:

13. Prasana Sahoo, S. Dhara, S. Amirthapandian, A. K. Tyagi, *Role of incubation time on the nucleation mechanism of square, hexagonal, and triangular biphase homostructure in GaN nanowires.* (Manuscript under Preparation).

Conference Proceeding:

1. P. S. Murthy, Prasana Sahoo, V. P. Venugopalan, S. Dhara, G. Saini, A. Das, A. K. Tyagi, *Ga2O3 Nanoparticles Inhibit Bacterial Adhesion & Biofilm Formation,* IEEE Xplore, Proc. of the "International Conf. on Nanoscience, Engineering and Technology" (ICONSET-2011), Chennai, 2011, 490-493, 978-1-4673-0074-2111.

2. Prasana Sahoo, S. Dhara, A. Patsha, S. Dash, M. Kamruddin, A. K. Tyagi, *Catalysis Free Growth Of GaN Nanostructures,* DAE Solid State Physics Symposium (DAE-SSPS-2011), Chennai, AIP Conf. Proc. 2011, 1447, 449-450; doi:http://dx.doi.org/10.1063/1.4710073

3. A. Patsha, Prasana Sahoo, S. Dhara, A. K. Tyagi, *Self-catalyzed Anisotropic Growth Of GaN Spirals*, DAE Solid State Physics Symposium (DAE-SSPS-2011), Chennai, AIP Conf. Proc., 2011, 1447, 1289-1290; doi:http://dx.doi.org/ 10.1063/1.4710484.

4. A. Patsha, Prasana Sahoo, S. Dhara, A. K. Tyagi, *Growth of GaN nanostructures on graphene*, IEEE Xplore, Proc. of the "International Conf. on Nanoscience, Engineering and Technology" (ICONSET-2011), Chennai, 2011, 553-555, DOI: 10.1109/ICONSET.2011.6168029

Conference Presentations:

1. Prasana Sahoo, P. Sriyutha Murthy, S. Dhara, V. P. Venugopala, S. Dash, A. K. Tyagi, *Probing the Dynamics of Cellular Damage in Bacterial Cells Induced by GaN Nanoparticles using Confocal Laser Raman spectroscopy,* Inter. Conf. Nanoscience & Technology (ICONSAT), 2012, Hyderabad. [Best Paper Awarded]

2. Avinash Patsha, Prasana Sahoo, S. Dhara, A. K. Tyagi, *Probing crystallographic orientation of GaN nanotube by polarized Raman spectroscopy,* 23rd International Conference on Raman Spectroscopy (ICORS), IISC, Bangalore (Accepted).

3. Prasana Sahoo, S. Sumathi, S. Dhara, S. Bera, S. Rangarajan, S. Dash, A. K. Tyagi, B. Raj, *"Functional GaN nanowires for label-free Genosensor"* 3rd Bangalore Nano, Bangalore, India.

4. Prasana Sahoo, Sandeep K., Soumee Chakraborty, S. Dhara, A. Das, S. Dash, A. K. Tyagi, B. Raj, *"Functionalization of GaN nanowires for label-free biomolecule detection",* India-Brazil-South Africa (IBSA) Nanotechnology School on Advanced Materials, 2010, Chennai.

5. Prasana Sahoo, S. Dhara, S. Dash, A. K. Tyagi & B. Raj, *"Surface optical Raman modes of single GaN belt"*, ICONSAT, 2010, IIT-Bombay.

6. Prasana Sahoo, S. Dhara, S. Dash, A. K. Tyagi & B. Raj, *"Large Scale Vapor- Phase Synthesis of Gallium Nitrides Nanobelts"*, International Workshop on Nanotechnology and Advanced Functional Materials (NTAFM), 2009, Pune (*Contributory presentation*).

7. Prasana Sahoo, S. Dhara, S, Dash, A. K. Tyagi, *"Growth of GaN Microbelt for Advanced Applications",* STEM-2010, Anupuram.

8. S. Dhara, Prasana Sahoo, and A. K. Tyagi, *"III-V Nitride Nanostructures: Nanoelectronics",* National Conference on Future Trends in Information & Communication Technology & Applications-2011, Bhubaneswar.

Workshop/Training

1. Cancer Nanotechnology, 2010, IIT-Bombay

2. Indian Nanoelectronics User Program (INUP) and device fabrication, 2009, IIT- Bombay.

3. Indo- US Workshop in "Visible and Ultra violate sources for Solid State Lightening and Water purification", 2009, Anna University, Chennai.

4. "Quantum condensed matter system" 2008, Institute of Mathematical Science, Chennai.

Name   :   **R. Kamala Kannan**
Enrolment No.   :   PHYS02200704002
Constituent Institute   :   Indira Gandhi Centre for Atomic Research, Kalpakkam
Title   :   Synthesis and Characterization of Few Walled Carbon
                                  Nanotubes and Studies for Gas Sensor Applications

Abstract

CNT based research have come a long way since its celebrated discovery by Iijima in 1991. Applications based on CNTs have been demonstrated in the field of sensors, solar cells, thin film transistors and medicine. However, still it is too far for this material to reach in the hands of common man as a utility in our day to day life. In this context the study of this material comes in to prominence as to address the issues pertaining to mass production, characterization and implementation in technological applications.

CNTs are hollow nanostructure can exist as single tube known as single walled CNT (SWCNT) or in the form concentric tubes known as multiwall CNT (MWCNT). The structure is one dimensional with axial symmetry exhibiting a spiral conformation called chairality. The quantum mechanical confinement of electrons around the circumference of the tube determines the nature of the tube as metallic or semiconducting. Irrespective of the chirality, a number of modes available for conduction of electrons govern the transport properties that strongly depend on tube diameter. In view of this, FWCNTs are a special type of small diameter multi-walled carbon nanotube with superb structural perfection. FWCNT are consists few layers of tubes or less than 10 nm in diameter.

The choice of FWCNT in the current study is owing to its unique features. FWCNT has a narrow band gap and easy to synthesize and scale up compared to SWCNTs. High structural stability under large current flow and protected inner wall from chemical modifications are important consideration for technological applications. A combination of these properties ensures reduction in failure of electronic devices, compatibility to functionalization and decoration without affecting the integrity of the tubes. In this thesis, we adapt a comprehensive approach to understand this wonderful material by going through the three important steps like synthesis, characterization and application.

In nutshell, this thesis investigates the CNT growth process by CVD using two catalytic support materials using a home built TGA-MS system. An extensive characterization is carried out using SEM, TEM, Raman and FTIR spectra to study FWCNTs microstructure. Temperature dependent electrical transport measurements are carried out and the observed electrical conductivity is modeled with a combination of VRH and FIT mechanism. It is found that transport property of a random network depends on the structural property of the constitutent FWCNTs. The possibility and potential advantage of developing gas sensor with SnO_2 and Pd decorated FWCNT is demonstrated. The field emission properties are studied and analyzed with F-N equation.

Publications

Peer reviewed Journals

1. R. Kamalakannan, K. Ganesan, S. Ilango, N. Thirumurugan, V. N. Singh, M. Kamruddin, B. R. Mehta, and A. K. Tyagi. The role of structural defects on the transport properties of a few-walled carbon nanotube networks, Appl. Phys. Lett. 98, 192105 (2011).

2. R. Kamalakannan, K. Ganesan, M. Kamruddin, and A. K. Tyagi. Temperature Dependent Transport Properties of a Few-walled Carbon Nanotubes Network, AIP Conf. Proc. 1313, 215 (2010).

3. R. Kamalakannan, S. Ilango, M.Kamruddin and A.K. Tyagi. The Effect of Catalyst on Synthesis of Carbon Nanotubes: An In Situ TGA Study, AIP Conf. Proc. 1447, 303 (2012).

4. R. Kamalakannan, S. Karthika, M. Kamruddin and A. K. Tyagi. Pd decorated few walled carbon nanotube networks for room temperature hydrogen sensor applications, IEEE Conf Proc. 559, (2011).

5. R. Kamala kannan, P. Jeyaraman, P.K. Ajikumar, S. Ilango, M. Kamruddin and A.K. Tyagi. Effect of catalyst supports in the synthesis of carbon nanotube using methane by chemical vapor deposition (communicated).

6. R. Kamalakannan, S. Ilango, S. Amirthapandian, M. Kamruddin and A. K. Tyagi. Incorporation of selectivity in Discrete SnO2 decorated few walled CNTs for gas sensing applications (communicated).

7. R. Kamala Kannan, George Joseph, P. Shankar, R.V. Subba Rao, A.K. Tyagi, P.R. Vasudeva Rao. Neutron absorber coatings for criticality control in annular tanks employed in spent fuel reprocessing, Annals of Nuclear Energy 36, 1211 (2009). 170

8. R. Kamalakannan et al., Raman spectroscopy on evaluation of FWCNTs during purification (Under preparation).

Conferences

1. R. Kamalakannan, Kalpataru Panda, B.Sundaravel, V.Thomas Paul, M.Kamruddin, A.K.Tyagi. Synthesis of helical carbon nanotubes and their field emission characteristics, International Conference on CarbonNanotechnology-2010, IITK, India.

2. R. Kamalakannan, K. Aruna, S. Ilango, M.Kamruddin, and A.K.Tyagi. A novel method of cap removal to enhance structural perfection in few walled carbon nanotubes, International Conference on Electron Nanoscopy-2011, Hyderabad, India.

3. R. Kamalakannan, M. Kamruddin and A.K. Tyagi. Synthesis of Metal FillednCarbon nanotube towards sensor applications, Nano Sensors 2008- Nationaln workshop on Nano Sensors & Devices, IIT Delhi, India.

4. R. Kamalakannan, P. Jeyaraman, Priyadharsini, P. K. Ajikumar, Chittaranjan Das, M. Kamruddin and A. K. Tyagi. Effect of zeolite and MgO template for CNT growth using CH4 feed stock by TCVD, India-Brazil-South Africa (IBSA) Nanotechnology School on Advanced Materials-2010, Kalpakkam, India.

5. R. Kamala kannan, M. Kamruddin and A. K. Tyagi. Effect of support and catalyst on CNT growth using CH4 feed stock by TCVD, ICONSAT-2010, IITB, India.

6. M. Kamruddin, Sathya Priya, R Kamalakannan, P K Ajikumar and A K Tyagi. Effect of synthesis method and conditions on ZnO nanostructures, CONSAT-2010,IITB, India.

Name	:	**Atindra Mohan Banerjee**
Enrolment No.	:	CHEM01200604010
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Synthesis, Characterization and Catalytic Activity of Novel Mixed Oxides for Energy and Environmental Related Reactions

Abstract

The main focus of this thesis is invoking the use of mixed oxide based heterogeneous catalysts for the two hydrogen production processes – thermochemical and photocatalytic. Iron oxide based catalysts have been investigated in detail for sulphuric acid decomposition reaction – the most endothermic step of sulphur based thermochemical water splitting cycles. The various iron oxide based powder samples viz. Fe_2O_3, doped Fe_2O_3, AFe_2O_4 ($A=Cu^{2}+$, $Co^{3}+$ and $Ni^{2}+$) were synthesized by ceramic as well as softer routes like gel combustion, co-precipitation and characterized for structure, morphology, redox properties, oxidation states by XRD, N_2-BET surface area, FTIR, TPR/O, XPS and SEMDAX. The catalytic activities of these oxides were evaluated in an indigenously developed flow through quartz catalytic reactor for sulfuric acid decomposition. Further, the compositions Fe_2O_3 and $Fe_{1.8}Cr_{0.2}O_3$ along with a commercial Pt/Al_2O_3 catalyst were evaluated as a catalyst at larger scale (~20 g) in granular from as a function of temperature (700-825 °C), time (~100h) and sulfuric acid flux (0.2-10 ml/min) in an indigenously constructed intergrated boiler, per-heater and catalystic decomposer. Ex-situ catalyst investigation suggested that the enhanced catalytic activity of Cr0doped Fe_2O_3 can be ascribed to the lower thermal stability of its sulfate and improved redox properties. On the other hand the Pt/Al_2O^3 catalyst suffered from substrate phase changes, substrate sulfation, decrease in porosity and surface area of support and Pt-particle agglomeration. On the basis of the studies carried out in this thesis the composition $Fe_{1.8}Cr_{0.2}O_3$ was peoposed to be a suitable substitution for noble metal based catalyst for sulfuric acid decomposition reaction Subsequently, $Fe_{1.8}Cr_{0.2}O_3$ catalyst is being tested at in closed loop decomposition plant of Sulfur-Iodine cycle. Chemical Technology Division, BARC. The most probable mechanism of sulfuric acid decomposition over the iron oxide based catalyst was also proposed.

Indium Titanate (In_2TiO_5) based system was investigated for photocatalytic hydrogen generation in water-methanol mixtures. Samples were prepared by solid-state, polyol and solvothermal routes to investigate the effect of morphology on photocatalystic activity. The high photocatalytic activity of In_2TiO_5 is attributed to its favourable electronic structure and crystal structure. Effect of Ni-doping at the A-site of In_2TiO_5 on the photocatalytic activity and redox properties was also investigated. The higher photoactivity of Ni-doped samples was attributed to better light absorption properties.

Publications

Journal Publications:

1. M. Banerjee, M. R. Pai, K. Bhattacharya, A. K. Tripathi, V. S. Kamble, S. R.Bharadwaj and S. K. Kulshreshtha Catalytic Decomposition of Sulfuric Acid on Mixed Cr/Fe Oxide Samples and its Application in Sulfur–Iodine Cycle for Hydrogen Production, *nternational Journal of Hydrogen Energy* 33 (2008) 319-326.

2. A. M. Banerjee, M. R. Pai, S. S. Meena , A. K. Tripathi and S. R. Bharadwaj, Catalytic Activities of Cobalt, Nickel and Copper Ferrospinels for Sulfuric Acid Decomposition: The High Temperature

Step in Sulfur Based Thermochemical Water Splitting Cycles, *International Journal of Hydrogen Energy* 36 (2011) 4768.

3. A. M. Banerjee, M. R. Pai, S. R. Bharadwaj, Influence of Ni Substitution on Redox Properties of $In_{2(1-x)}Ni_{2x}TiO_{5-\delta}$, *Thermochimica Acta* 516 (2011) 40–45.

4. M. R. Pai, A. Singhal, A. M. Banerjee, R. Tiwari, G. K. Dey, A. K. Tyagi, S. R. Bharadwaj, Synthesis, Characterization and Photocatalytic H2 generation over Ternary Indium Titanate Nanoparticles, *Journal of Nanoscience and Nanotechnology* 11 (2012) 1-10.

5. Mrinal R. Pai, Jerina Majeed, Atindra M. Banerjee, Ashok Arya, Shovit Bhattacharya, Rekha Rao, and Shyamala R. Bharadwaj, Role of Nd^{3+} Ions in Modifying the Band Structure and Photocatalytic Properties of Substituted Indium Titanates, $In_{2(1-x)}Nd_{2x}TiO_5$ Oxides, *Journal of Physical Chemistry C* 116 (2012) 1458-1471.

6. M. R. Pai, A. M. Banerjee, S. R. Bharadwaj and S. K. Kulshreshtha, Synthesis, Characterization, Thermal Stability and Redox Behavior of $In^{3+}{}_2Ti^{4+}{}_{1-x}Tm^{3+}{}_xO_{5-\delta}$ (Tm = Fe^{3+} and Cr^{3+}, $0.0 \leq x \leq 0.2$) Mixed Metal Oxide Catalysts, J of Mater. Res., 22 (2007) 1787.

7. A. M. Banerjee, A. R. Shirole, M. R. Pai, A. K. Tripathi, S. R. Bharadwaj, D. Das, P. K.Sinha, Catalytic Activities of Fe_2O_3 and Chromium Doped Fe2O3 for Sulfuric Acid 241 Decomposition Reaction in an integrated boiler, preheater and catalytic decomposer, *Applied Catalysis B: Environmental,* 127 (2012) 36-46.

8. A. M. Banerjee, M. R. Pai, S. R. Bharadwaj, Role of Ni substitution on photocatalytic properties of In2TiO5, *Journal of Materials Research*, *to be communicated*

9. A. M. Banerjee, M. R. Pai, A. K. Tripathi, S. R. Bharadwaj and D. Das, Catalytic decomposition of sulfuric acid over Pt/Al2O3 catalysts in pellet form, *manuscript under preparation.*

Books:

1. Mrinal R. Pai, Atindra M. Banerjee, A. K. Tripathi and Shyamala R. Bharadwaj, authored Chapter 14 titled "Fundamentals and Appplications of the Photoctalytic Water Splitting Reaction", in book "*Functional Materials: Preparations, Processing and Applications*" edited by S. banerjee and A. K. Tyagi, published by Elsevier Insights, USA, 2012, pg. 579- 606.

Journal Publications (Other than thesis, in related field):

1. K. K. Kartha, M. R. Pai, A. M. Banerjee, R. V. Pai, S. S. Meena and S. R. Bharadwaj, Modified Surface and Bulk Properties of Fe-Substituted Lanthanum Titanates enhances Catalytic activity for CO+N_2O reaction, J. Molec. Catal. A, 335 (2011) 158–168.

2. M. R. Pai, A. M. Banerjee, K. Karha, R. V. Pai, V. S. Kamble, S. R. Bharadwaj, Mechanism of CO + N_2O Reaction via Transient CO_3^{2-} Species over Crystalline Fe- Substituted Lanthanum Titanates, J. Phys. Chem. B, 114 (2010), 6943–6953.

Symposium/Conferences/Research Scholars Meet/School:

1. M. Banerjee, A. R. Shirole, M. R. Pai, A. K. Tripathi, S. R. Bharadwaj and D. Das, Kinetics of sulfuric acid decomposition over iron oxide based catalysts, presented in Joint IAEA – ICTP Advanced School on "Development and characterization of materials for hydrogen-based energy systems: Role of nuclear technology" held at International Centre for Theoritical Physics (ICTP), Trieste, Italy on 13-18 June 2011.

2. A. M. Banerjee and S. R. Bharadwaj, "Studies on Catalysts for Sulfuric Acid Decomposition Reaction", presented orally at Research Scholars Meet - 2011 held during Feb-2011 organized by Indian Chemical Society.

3. A. M. Banerjee, A. R. Shirole, M. R. Pai, A. K. Tripathi and S. R. Bharadwaj, "Synthesis, characterization and Catalytic Activity of Mixed Metal Oxides for Energy and Environment Related Reactions" presented orally at CATSCHOL-2011 ICT, Mumbai Mar-2011.

4. A. M. Banerjee, A. R. Shirole, M. R. Pai, A. K. Tripathi, S. R. Bharadwaj and D. Das Catalytic decomposition of sulfuric acid over Fe_2O_3 and Pt/Al_2O_3: A comparative study"poster presentation at 3rd DAE-BRNS ISMC-2010 held at BARC, Mumbai on 7-11th Dec 2010.

5. A. M. Banerjee, A. R. Shirole, M. R. Pai, A. K. Tripathi, V. S. Kamble, S. R. Bharadwaj, D. Das, P. K. Sinha "Catalytic decomposition of sulfuric acid: an important step in sulfur-iodine thermochemical cycle for hydrogen generation using nuclear heat from CHTR", Poster presentation at Peaceful Uses of Atomic Energy (PUAE-09) held in Delhi during 29th Sept to 1st Oct 2009. AR-8 pp. 250-251.

6. A. M. Banerjee, M. R. Pai, A. K. Tripathi and S. R. Bharadwaj on "Application of transition metal ferrites AFe_2O_4 (A= Co, Ni, Cu) for the catalytic decomposition of sulphuric acid involved in Sulphur-Iodine Thermochemical Cycle for Nuclear Hydrogen production" was presented at Peaceful uses of atomic energy (PUAE-09) held in Delhi during 29th Sept to 1st Oct 2009.

7. A. M. Banerjee, A. R. Shirole, M. R. Pai, A. K. Tripathi, V. S. Kamble, S. R. Bharadwaj and D. Das "Studies on sulfuric acid decomposition over iron oxide catalyst" was presented at World Hydrogen Technologies Convention, (WHTC-09) held at New Delhi on 26-28 Aug' 2009.

8. M. R. Pai, Atindra M. Banerjee, Jerina Majeed, Shyamala. R. Bharadwaj on "Photocatalytic Water Splitting Reaction under actual Sun Light/Sunlight-type Irradiation using Substituted Indium Titanates, $In_{2(1-x)}A_{2x}Ti_{1-y}Tm_yO_5$ (A = Ni^{2+} and Nd^{3+}, Tm = Fe^{3+} and Cr^{3+}, x/y=0.0-0.2)" was presented at World Hydrogen Technologies Convention, (WHTC- 09) held at New Delhi on 26-28 Aug' 2009.

9. A. M. Banerjee, A. R. Shirole, K. Bhattacharyya, M. R. Pai, S. Varma, A. K. Tripathi, V. S. Kamble, S. R. Bharadwaj, S. R. Nair, P. K. Sinha and D. Das, Results on long term catalytic activity of iron oxide for decomposition of sulfuric acid" poster presentation in SMC-2008 held at BARC, Mumbai on 2-6th Dec 2008.

10. A. M. Banerjee, M. R. Pai, and S. R. Bharadwaj, Preparation and characterization of mixed oxides for environmental and energy related reactions; oral presentation in National Symposium for Materials Research Scholars- MR08, held at Indian Institute of Technology, Powai, Mumbai on 17th-18th May (2008) 42.

11. A. M. Banerjee, M. R. Pai, and S. R. Bharadwaj; Temperature programmed reduction of $In_{2(1-x)}Ni_{2x}TiO_{5-\delta}$ oxides; oral presentation in Sixteenth national Symposium on Thermal Analysis (THERMANS-2008) at IGCAR, Kalpakkam, Feb 4-6, (2008), 293-295.

12. A. M. Banerjee, M. R. Pai, K. Bhattacharya, A. K. Tripathi, V. S. Kamble, S. R. Bharadwaj, S. K. Kulshreshtha, "Studies on sulfur-iodine thermochemical cycle for hydrogen production" poster presentation in the 3rd DAE-BRNS ISMC-2010 held at BARC, Mumbai on 7-11th Dec 2010.

Awards:

1. One of the recipient of DAE Group Achievement Award 2010, titled "Development of Catalysts for Various Applications Related to DAE Programme"

2. Best Paper Award (third) for poster presentation: A. M. Banerjee et al for "Studies on Sulfur-Iodine Thermochemical cycle for Hydrogen Production" in ISMC-2006 held at BARC, Mumbai on Dec 2006.

3. Best Paper Award (Second) for oral presentation: A. M. Banerjee et al for "Preparation and characterization of mixed oxides for environmental and energy related reactions" in National Symposium for Materials Research Scholars- MR08, held on 17th- 18th May, 2008 at Indian Institute of Technology, Bombay.

4. Best Paper Award (Second) for oral presentation: A. M. Banerjee et al for "Temperature programmed reduction of In2(1-x) Ni2xTiO5-d oxides" in Sixteenth national Symposium on Thermal Analysis (THERMANS-2008) at IGCAR, Kalpakkam, Feb 4-6, 2008.

5. Best Paper Award (Second) for poster presentation: A.M. Banerjee et al for "Catalytic decomposition of sulfuric acid over Fe2O3 and Pt/Al2O3: comparative study" in ISMC-2010 held at BARC, Mumbai on 7-11th Dec 2010.

Name	:	**Charu Dwivedi**
Enrolment No.	:	CHEM01200704001
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Development of Novel Sorbent Beads for Removal of Radionuclides and Organic Contaminants

Abstract

Among the various processes used in water and wastewater treatment, adsorption has been proved to be an excellent way, to treat industrial waste effluents, offering significant advantages like the low-cost, availability, profitability, easy operation and efficiency. Several materials, such as activated carbon, chelating resins, clays, functionalized silica, etc., have been studied for removal toxic metal ions from aqueous solutions (1). Most of the commercialized adsorbents are organic resins, but these have their own limitations, such as poor thermal & radiation stability and mechanical strength. Whereas inorganic adsorbents have high chemical and radiation stability, but because of their fine morphology, or gel like nature, these create excessive pressure drops across the fix bed and low hydraulic conductivity and hence cannot be used as such in any flow-through systems(2). Moreover, the fine powdery inorganic adsorbents, generated from granular particles during purification process, remain suspended in the water, and act as contaminants. The above limitations of organic resins and inorganic sorbents could be overcome by introducing composite resins consisting o inorganic sorbents and organic binding matrices.

Here, we have developed a technique based on phase inversion, to synthesize adsorbent-polymer composites, containing different potential inorganic adsorbents, such as manganese dioxide, copperhexacyanoferrate, ferric hydroxide, and titanium dioxide, using polymers, like polyacrylonitrile and polyethersulfone. Suitable size and mechanical stability, along with their spherical shape, make these composites most appropriate for column operation. These synthesized polymer-adsorbent composites have been thoroughly characterized, using FTIR, TGA-DSC and XRD techniques. These composite materials have shown potential for removal of toxic metal from aqueous medium.

Publications

Patent

1. A new method for synthesis of resol beads with good control over their size C. Dwivedi, K. K. Singh, M.Kumar, I. J. Singh, P. N. Bajaj, Patent Application submmited (2012).

Journal

1. Resorcinol-Formaldehyde Coated XAD Resin Beads for Removal of Cesium Ions from Radioactive Waste: Synthesis Adsorption and Kinetic Studies C. Dwivedi, A. Kumar, K. A. Juby, K. K. Singh, M. Kumar, P. K. Wattal, P. N. Bajaj, *RSC Advances* 2012, 2, 5557-5564.

2. Synthesis and Characterization of Mesoporous Titania Microspheres and their Applications C. Dwivedi, N. Raje, J. Nuwad, M. Kumar, P. N. Bajaj, *Chemical Engineering Journal*, 2012, 193–194, 178-186.

3. Preparation and Evaluation of Alginate Assisted Spherical Resorcinol- Formaldehyde Resin Beads for Removal of Cesium From Waste C. Dwivedi, A. Kumar, K. A. Juby, M. Kumar, P. K. Wattal, P. N. Bajaj, *Chemical Engineering Journal*, 2012, 200-202, 491-498.

4. Copperhexacyanoferrate-Polymer Composite Beads for Cesium Ion Removal: Synthesis, Characterization, Sorption and Kinetic Studies C. Dwivedi, A. Kumar , K. A. Juby, K. K. Singh, M. Kumar, P. K. Wattal, P. N. Bajaj, *Journal of Applied Polymer Science,* 2012, DOI: 10.1002/app.38707.

5. Removal of Cesium by Spherical Resorcinol-Formaldehyde Resin Beads: Sorption and Kinetic Studies C. Dwivedi, S. K. Pathak, M. Kumar, S. C. Tripathi, P. N. Bajaj, *Journal of Radioanalytical and Nuclear Chemistry*, 2012, DOI 10.1007/s10967-012-2320-y.

6. Uptake Studies of Arsenic [(III) and (V)] on Synthesized Mesoporous Titania Microspheres C. Dwivedi, N. Raje, M Kumar, A. V. R. Reddy, P. N. Bajaj, *Journal off Radioanalytical and Nuclear Chemistry* 2012, 294, 131-136.

7. Preparation and Characterization of Potassium Nickelhexacyanoferrate Loaded Hydrogel Beads for the Removal of Cesium Ions C. Dwivedi, S. K. Pathak, M. Kumar, S. C. Tripathi, P. N. Bajaj, (Communicated, 2012).

8. Potassium copperhexacyanoferrate-Hydrogel Beads: Synthesis, Characterization and Applications C. Dwivedi, S. K. Pathak, M. Kumar, S. C. Tripathi, P. N. Bajaj, (To be communicated, 2012).

9. Selective Removal of Cesium Ions by Potassium Cobalthexacyanoferrate-Gel beads: Kinetics, and Sorption Isotherms Studies C. Dwivedi, S. K. Pathak, M. Kumar, S. C. Tripathi, P. N. Bajaj, (To be communicated, 2012).

Name	:	**Sita Sundar**
Enrolment No.	:	PHYS06200704010
Constituent Institute	:	Institute for Plasma Research, Gandhinagar
Title	:	Study of Fast Time Scale Phonomena in Plasmas

Abstract

Plasma is a very complex medium. A typical plasma medium is a charged manybody system which generates and responds to electromagnetic fields and behavesin a collective fashion. Often, simplifications in such a complex plasma system are desirable. A gross simplification is possible by adopting a macroscopic flui picture wherein properties averaged over a large number of particles constitute a small fluid element whose propagation can be followed up in space and time. Furthermore, due to the huge difference in the masses of the constituent species of the plasma (ions are typically 1840 times heavier than electrons), their response times are very different. Hence, a further simplification is possible if the phenomena under consideration falls under the time scale regime where only one of the constituent regime can have a dominant response. The exploitation of such time scale separation has led to various simplified models for plasma depiction. Based on the idea of the exploitation of time scale separation, plasma phenomena can be broadly categorized into two groups: (a) Slow ion time scale phenomena, where one can assume instantaneous response of electrons and (b) fast electron time scale phenomena, for which ions are assumed to provide merely a stationary neutralizing background. In both the regimes of (a) and (b) further simplifications are possible and have been adopted in literature, based on more definite information about the phenomena under consideration. While the regime of ion response has been studied extensively since almost a century and interesting studies are still being pursued in this area, the phenomena associated with fast electron time scale response has been relatively less explored. It is only recently (with the advent of fast high power lasers) that the laboratory plasma can be triggered to respond and diagnosed at these time scales, and studies in this regime have gained prominence.

We have chosen to investigate some fundamental issues which also have practical relevance in the regime of fast electron time scale response in plasmas. In particular, the thesis explores the electron shear flow driven instabilities and coherent nonlinear solutions that may form in this domain of plasma response. The magnetized and relativistic nature of the electron fluid produces interesting features in the electron shear flow driven Kelvin - Helmholtz (KH) like mode of the plasma. The study concerning this instability has been presented in the part - I of the thesis. In part - II, the study of the existence of nonlinear coherent structure in the coupled laser plasma system has been presented. The dynamical evolution of some of the solutions and questions pertaining to the stability of some of these structures have also been looked at.

The sheared electron flow in the non-relativistic regime has often been described by a reduced fluid Electron Magnetohydrodynamic (EMHD) model. EMHD model describes the dynamics of magnetized electron fluid in the presence of self-consistent and external electric and magnetic field on time scales in between electron and ion gyrofrequencies. Here, ion dynamics is completely ignored and role of ions is simply to provide neutralizing background. The electron fluid is assumed to be incompressible in this limit, the density perturbations as well as the displacement current are assumed to be negligible in this case.

The EMHD model resembles closely the neutral hydrodynamic fluid system and hence the characteristic neutral fluid instabilities are also present here as well, albeit with appropriate modifications due to magnetized character of the electron fluid. The distinction and similarities of the KH mode in neutral fluid and the EMHD has been outlined in the past by several authors. The sheared flow of electrons also constitutes a sheared current in the plasma. It has so far not been clear, which between the two, the current shear or the velocity shear, was responsible for the instability of sheared electron flow configuration. It is for this reason that this mode has often been also referred to as the sausage and/or kink mode [1, 2], the nomenclature used when the current shear produces instability in a plasma. We have employed a generalised Electron Magnetohdrodynamic description to distinguish a sheared current flow configuration from the case with velocity shear, by choosing an appropriately tailored inhomogeneous electron density profile. The instability studies carried out for the two configuration then clearly shows that in 2-D the instability is driven by the shear in electron flow velocity, and hence it is a KH like mode. The interpretations for certain characteristic features, such as existence of a threshold wavenumber along the flow direction and the excitation of sharper scales in the direction normal to both shear and flow directions, the order of magnitude estimation of the growth rate etc., from physical considerations of the release in the free energy source has also been provided by us.

An important practical implication of the KH instability driven by a sheared electron current flow can be in the context of fast ignition (FI) mechanism of laser fusion [1–6]. The FI is a variant of the inertial confinement fusion scheme in which the task of material compression is separated from that of ignition by employing two separate laser pulses. While the compression is done by a slow nanosecond laser pulse, for ignition one employs a fast sub-picosecond laser. The gnitor pulse is unable to penetrate the overdense compressed target core and instead produces hot energetic electrons which propagate towards the compressed target core. It is desirable that these energetic electrons dump their energy in the compressed core of the target to produce the hot spot for ignition. The transport of energetic electrons in the plasma, is therefore an important issue. The flow of energetic electrons is typically countered by reverse shielding current provided by the background plasma immediately. The forward and background currents, upon suffering Weibel, tearing and coalescence instability produce cylindrical current channels. The central portion of which carries the forward current and the external cylindrical shell carries the reverse shielding current. The flow of electrons in the cylinder along its axis, therefore, has sufficient shear in the radial direction. This sheared flow configuration would in general be susceptible to the KH instability. However, since the energetic electron flow can be relativistic, it is important that the relativistic effects on the EMHD KH mode be understood. For this purpose, we have carried out a detailed investigation of the KH mode in the relativistic regime.

Our studies on the KH mode for the sheared electron flow which is relativistic reveals that there are characteristic differences with the nonrelativistic case. We have shown that the incorporation of displacement current (as the flows are now relativistic) has little influence on the mode. However, as the relativistic mass factor can also be sheared, we observe that the possibility of exciting modes sharper than the velocity shear scale in the flow direction exists. We also show that the unstable domain of the wave-number space is considerably wider in this case and the mode does not remain purely growing but acquires a real frequency even for a purely antisymmetric velocity profile. We have provided an understanding of these features observed in the strongly relativistic regime as resulting from the shear in the relativistic mass factor γ.

The results of the weakly relativistic case observed from numerical analysis has also been reproduced by a perturbative analytic treatment. A good matching between the numerical exact results for the maximum growth rate and the threshold wave vector has been demonstrated by us.

We notice that for solutions moving with the group velocity of ⧫ = 0 and/or very small, the assumption of static ions should not be made. We, therefore incorporated the effect of ion dynamics and investigated the eigen spectra afresh. We notice several additional new varieties of solitonic structures in this case. We also observe that the bright soliton solutions (with light pulse trapped within the central

region) are not permitted at low group velocities in this case. Instead dark solitonic structures can form. At the edge, a particular variety of flat top solutions are shown to exist.

A detailed dynamical evolution of the flat top solutions have also been carried out. The studies show that the flat top solutions propagate stably for several plasma periods. However, they are observed to be susceptible to an instability, which has been identified as the backward Brillouin instability process. In the cold plasma, it is a quasi-mode where the role of temperature is played by the electron quiver velocity.

Further extension of our work in both the problems can be carried out. The linear analysis of the relativistic flow shear driven instability in EMHD is useful in understanding the basic physics of the excitation of the unstable mode but nonlinear studies are very important. With the nonlinear studies we will be able to have deeper insights regarding the evolution properties, saturation etc. The nonlinear studies of the relativistic EMHD mode would be crucial for the estimation of the effective transport properties of the electron flow. This is specially pertinent, as pointed out by us, in the context of FI concept of laser fusion.

The dynamical evolution of flat-top solitons has shown that they develop a backward Brillouin scattering instability. It would be interesting to see how some of the stable structures behave when the two-dimensional perturbations allow for a side scattering process. The three-dimensional generalization, the effect of relativistic temperature on the stability properties and dynamics of electromagnetic solitons are other issues of interest for future investigation.

Publications

Publications in Peer Reviewed Journals:

1. Detailed Characterization of Relativistic Electromagnetic Solitons in Cold Plasma , Sita Sundar and Amita Das Physics of Plasmas (to be submitted).

2. Perturbative analysis of sheared flow Kelvin-Helmholtz instability in a weakly relativistic magnetized electron fluid, Sita Sundar, Amita Das, and Predhiman Kaw Physics of Plasmas 19, 052105 (2012).

3. Relativistic electromagnetic flat top solitons and their stability, Sita Sundar, Amita Das, Vikrant Saxena, Predhiman Kaw, and Abhijit Sen Physics of Plasmas 18, 112112 (2011).

4. Free energy source for flow shear driven instabilities in electronmagnetohydrodynamics, Sita Sundar and Amita Das Physics of Plasmas 17, 042106 (2010).

5. Electron velocity shear driven instability in relativistic regime, Sita Sundar and Amita Das Physics of Plasmas 17, 022101 (2010).

6. Role of natural length and time scales on shear driven two-dimensional electron magnetohydrodynamic instability, Gurudatt Gaur, Sita Sundar, SharadK.Yadav, AmitaDas, Predhiman Kaw, Sharveshwar Sharma Physics of Plasmas 16, 072310 (2009).

Name	:	**Arpita Datta**
Enrolment No.	:	CHEM02200704002
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	High Performance Separation Studies on Lanthanides and Some Actinides

Abstract

Lanthanides and actinides have many applications in diverse fields including nuclear industry. Individual separation of lanthanides and some actinides is challenging due to their same charge and similarity in size. The thesis is focused on the development of rapid separation methods for isolation of individual lanthanides and some actinides using various liquid chromatographic technique. In this context, individual separation of lanthanides and actinides was investigated on reversed phase chromatographic supports such as small particle (1.8 μm) and monolith based supports. A liquid chromatographic technique has been developed for the individual separation of lanthanides in about 2.7 min using a monolithic support. These methods were subsequently employed for the burn-up measurement on dissolver solutions of nuclear reactor fuels. A single stage dual column chromatographic technique was developed and demonstrated for the burn-up measurement on dissolver solution of PHWR (Pressurised Heavy Water Reactor, MAPS, Kalpakkam, India) and fast reactor fuel (FBTR, Kalpakkam, India). An HPLC technique has been developed for the estimation of lanthanide impurities in uranium matrix (1 in 10^5) using the dual column technique.

A method for the correction of retention of lanthanide and some actinide complexes with the stability constant was developed. The retention times as well as capacity factors of lanthanides and actinides were measured as a function of camphor-10-sulfonic acid (CSA), organic acid concentrations and mobile phase pH. Form these studies, a correlation has been established between capacity factor of a metal ion, concentrations of ion-pairing reagent and complexing agent with the stability constant of lanthanide/actinide complex. Using these methods, the estimation of stability constant of lanthanides and actinides was demonstrated with various ligands, e.g. hydroxyl isobutyric acid (α -HIBA), lactic acid, tartaric acid and mandelic acid. Seciation data for lanthanides, uranium, plutonium and americium with α -HIBA were computed. These studies were employed to explain the elution behavior of plutonium (various oxidation states), americium, uranium and thorium during reversed phase chromatography. The elution behavior of lanthanides was also investigated as a function of temperature using dynamic ion-exchange and reserved phase chromatographic techniques. The retention behavior of lanthanides and actinides was studied using task specific ionic liquids and individual separation of lanthanides and separation of uranium from thorium was demonstrated.

Publications

Journals

1. Rapid Separation of Lanthanides and Actinides on Small Particle Based Reverse Phase Supports; Arpita Datta, N. Sivaraman, T. G. Srinivasan and P. R. Vasudeva Rao; Radiochim. Acta, 98, (2010) 277-285.

2. Liquid Chromatographic Behaviour of Actinides and Lanthanides on Monolith Supports; Arpita Datta, N. Sivaraman, T. G. Srinivasan and P. R. Vasudeva Rao; Radiochim. Acta, 99, (2011) 275-283.

3. High Performance Separation and Supercritical Extraction of Lanthanides and Actinides; Arpita Datta, K. Sujatha, R. Kumar, N. Sivaraman, T. G. Srinivasan and P. R. Vasudeva Rao; Energy Procedia, Elsevier, 8, (2011) 425-430.

4. Single Stage Coupled Column HPLC Technique for the Separation and Determination of Lanthanides in Uranium Matrix-Application to Burn-up Measurement on Nuclear Reactor Fuel; Arpita Datta, N. Sivaraman, T. G. Srinivasan and P. R. Vasudeva Rao; Nuclear Technology (2013, TN-12-45).

5. Correlation of Retention of Lanthanide and Actinide Complexes with Stability Constant and Their Speciation; Arpita Datta, N. Sivaraman, K. S. Viswanathan, Suddhasattwa Ghosh, T. G. Srinivasan and P. R. Vasudeva Rao; Radiochimica Acta (0.1524/ract.2013.2005). 239

6. Influence of Temperature on the Elution Behaviour of Lanthanides and Some Actinides on Reversed Phase supports; Arpita Datta, N. Sivaraman, Suddhasattwa Ghosh, T. G. Srinivasan and P. R. Vasudeva Rao (manuscript to be submitted). National and International

Conferences

1. Retention Behaviour of Uranium and Thorium on N, N-di(2-ethylhexyl)isobutyramide= Reverse Phase Support; Arpita Datta, N. Sivaraman, T. G. Srinivasan and P. R. Vasudeva Rao; Nuclear and Radiochemistry Symposium (NUCAR-2009), Mumbai, India, p 487-488, 2009.

2. Task-Specific Ionic Liquids as Mobile Phase in Liquid Chromatography-Studies on the Sorption Behaviour of Uranium, Thorium and Lanthanides; Arpita Datta, N. Sivaraman, K. A. Venkatesan, T. G. Srinivasan and P. R. Vasudeva Rao, Nuclear and Radiochemistry Symposium (NUCAR-2009), Mumbai, India, p 489-490, 2009.

3. Liquid Chromatographic Behaviour of Actinides on Monolith Supports; Arpita Datta, N. Sivaraman, T. G. Srinivasan and P. R. Vasudeva Rao; Biennial Symposium on Separation Science and Technology (SESTEC-2010), Kalpakkam, India, p 463-464, 2010.

4. Fast Separation of Lanthanides and Actinides on Small Particle Support; Arpita Datta, N. Sivaraman, T. G. Srinivasan and P. R. Vasudeva Rao; Biennial Symposium on Separation Science and Technology (SESTEC-2010), Kalpakkam, India, p 465-466, 2010.

5. High Performance Separation and Supercritical Extraction of Lanthanides and Actinides; Arpita Datta, K. Sujatha, R. Kumar, N. Sivaraman, T. G. Srinivasan and P. R. Vasudeva Rao; 2nd International Conference on Asian Nuclear Prospects (ANUP-2010), Mamalapuram, India, p FR8, 2010.

6. Liquid Chromatographic Behavior of Lanthanides and it's Application on Burn-up Measurement; Arpita Datta, N. Sivaraman, T. G. Srinivasan and P. R. Vasudeva Rao; Nuclear and Radiochemistry Symposium (NUCAR-2011), Visakhapatnam, India, p 144- 145, 2011.

7. High Performance Separation Studies on Lanthanides and Actinides, Arpita Datta, N. Sivaraman, T .G. Srinivasan and P. R. Vasudeva Rao; Chemistry Research Scholar Meet (CRSM- 2011), Kalpakkam, India, 111, 2011.

8. Lanthanides and Actinides Separation Studies using Liquid Chromatography; Arpita Datta, N. Sivaraman, T. G.Srinivasan and P. R. Vasudeva Rao; International Conference on Vistas in Chemistry (ICVC-2011), Kalpakkam, India, p 30, 2011.

9. Separation and Estimation of Lanthanides using High Performance Liquid Chromatography; Arpita Datta, N. Sivaraman, and P. R. Vasudeva Rao; DAE-BRNS Theme Meeting on Recent trends in Analytical Chemistry (TRAC-2012), Chennai, India, p 54-55, 2012.

Award / Honors

1. Best oral presentation award in Nuclear and Radiochemistry symposium (NUCAR-2009) held at Mumbai, India.

2. Best Poster presentation award in DAE-BRNS Theme Meeting on Recent trends in Analytical Chemistry (TRAC-2012), held at Chennai, India.

Name	:	**Victor Roy**
Enrolment No.	:	PHYS04200704003
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	High Performance Separation Studies on Lanthanides and Some Actinides

Abstract

Recent experiments at the Relativistic Heavy Ion Collider (RHIC) at BNL and at the Large Hadron Collider at CERN have provided strong indications that in high-energy heavy ion collisions a strongly coupled Quark-Gluon-Plasma (QGP) is produced. This phenomenon gives us the unique opportunity to enhance our understanding of the physical properties (like transport coefficients) of this fundamental constituent of all visible matter. To this end we take phenomenological approach and have used a 2+1 dimensional causal relativistic viscous hydrodynamics to simulate the space-time evolution of the QGP and the subsequent hadronic phase. It is assumed that the fluid evolution follows longitudinal boost invariant flow profile for central rapidity region. The Equation of State (EoS) used in hydrodynamic simulation is constructed by parameterizing the resent lattice QCD data for high temperature QGP phase and form hadron resonance gas for low temperature hadronic phase. The effects of both bulk and shear viscosity on the fluid evolution as well as on the experimental observables has been studied. Where the viscous stresses were evolved according to the 2nd order causal theory given by Israel-Stewart (I-S) the invariant yield of charged hadron was calculated using Cooper-Frey formula. We have incorporated the dissipative correction to the equilibrium freeze-out distribution function following Grad's 14-moment method. The resonance decay contribution to the invariant yield of poin was also considered. The simulated results are then compared to experimental observables like invariant yield of all charged hadron, elliptic (V_2), and Hexadecapole flow (V_4) etc. to the shear viscosity of the QGP and hadronic phase.

We found that bulk viscous correction to the yield and elliptic flow of pion are too large validity of I-S theory breaks down. Particularly the main contribution of this large bulk viscous correction is coming from the correction in the equilibrium freeze-out distribution function. This is still an open issue. We have neglected the effect of bulk viscosity in the subsequent study when extracting shear viscosity from comparison of simulated results to the experimental observables. A detailed comparison of our simulated results from viscous hydrodynamics and experimental observables measured at RHIC and LHC indicates that the value of shear viscosity to density ratio (η / S) of the fluid produced in the heavy ion collision is very small. The estimated value of (η / S) from the RHIC and data have values in the range 1-4 times the lower limited ($1/4\pi$, in unit of h and c) of shear viscosity to entropy density predicted by a string theoretical calculation based on ADS/CFT. The small value of (η/s) estimated for the QGP formed in high-energy heavy ion collisions indicates that the system is strongly coupled, where the inter particle potential energy dominates over the (thermal) kinetic energy. In view of the extracted value of η/s, we can conclude that QGP is the most perfect fluid ever created by humankind in any laboratory experiment done so far.

Publications

1. 2+1 dimensional hydrodynamics including bulk viscosity: A Systematics study. Victor Roy, A.K. Chaudhuri. Published in Phys. Rev. C. 85 (2012) 024909.

2. Charged particle's elliptic flow in 2+1D viscous hydrodynamics at LHC ($\sqrt{s}NN$ = 2.76 TeV) energy in Pb+Pb collision. Victor Roy, A.K. Chaudhuri. Published in Phys. Lett. B 703 (2011) 313.

3. Elliptic flow of thermal dilepton as a probe of QCD matter. Payal Mohanty, Victor Roy, Sabyasachi Ghosh, Santosh K Das, Bedangadas Mohanty, Sourav Sarkar, Jane Alam, Asis K Chaudhuri. Published in Phys. Rev. C. 85 (2012) 031903.

4. Hydrodynamical analysis of centrality dependence of charged particle's multiplicity in √sNN = 2.76 TeV Pb+Pb collision. A.K. Chaudhuri, Victor Roy. Published in Phys. Rev. C . 84 (2011) 027902.

5. Hadronic resonance gas and charged particle's pT spectra and elliptic flow in √sNN = 200 GeV Au+Au collisions. Victor Roy, A.K. Chaudhuri. Published in Phys. Rev. C 82 (2010) 031901.

6. Transverse Momentum Spectra and Elliptic Flow in Ideal Hydrodynamics and Geometric Scaling. Victor Roy, A.K. Chaudhuri. Published in Phys. Rev. C 81 (2010) 067901.

7. Elliptic flow (v2) in pp collisions at energy available at the CERN Large Hadron Collider: A hydrodynamical approach. S.K. Prasad,Victor Roy, S. Chattopadhyay , A.K. Chaudhuri. Published in Phys. Rev. C 82 (2010) 024909.

8. Equation of state dependence of Mach cone like structures in Au+Au collisions. Victor Roy, A.K. Chaudhuri. Published in J.Phys.G 37 (2010) 035105.

Papers Communicated

1. Comparison of results from a 2+1D relativistic viscous hydrodynamic model to elliptic and hexadecapole flow of charged hadrons measured in Au-Au collisions at √sNN = 200 GeV. Victor Roy, A. K. Chaudhuri and Bedangadas Mohanty. Submitted to the Physical Review C. e-Print: arXiv:1204.2347.

2. Fluctuating initial condition and smoothening effect on elliptic and triangular flow. Md.Rihan Haque, Victor Roy, A. K. Chaudhuri. Submitted to the Physical Review C. e-Print: arXiv:1204.2986.

Conference proceedings

1. Transverse Momentum Spectra and Elliptic Flow in Ideal Hydrody- namics and Geometric Scaling. Victor Roy, A. K. Chaudhuri. Proceeding of the DAE Symp. On Nucl. Phys. 55 (2010) 582.

2. Lattice Based Equation and Transverse Momentum Spectra of Identified Particles in Ideal and Viscous Hydrodynamics. Victor Roy, A. K. Chaudhuri. Proceeding of the DAE Symp. On Nucl. Phys. 55 (2010) 624.

3. Charged particle pT spectra and elliptic flow in a 2+1D viscous hydro- dynamics including shear and bulk viscosity. Victor Roy, A K Chaudhuri. Proceeding of the DAE Symp. On Nucl. Phys. 56 (2011) 844.

4. Probing elliptic flow of QCD matter by lepton pairs. Payal Mohanty,Victor Roy, Sabyasachi Ghosh, Santosh K Das, Bedangadas Mohanty, Sourav Sarkar, Jan-e Alam, Asis K Chaudhuri. Proceeding of the DAE Symp. On Nucl. Phys. 56 (2011) 856.

5. Transport properties of the matter formed in heavy-ion collisions at the Large Hadron Collider. Victor Roy, A K Chaudhuri. Proceeding of the DAE Symp. On Nucl. Phys. 56 (2011) 910.

Name	:	**Arvind Kumar**
Enrolment No.	:	PHYS01200804026
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Growth Mode and Conduction Characteristics of Molecular Semiconductor Films

Abstract

In this thesis we have discussed the growth of mononuclear cobalt phthalocyanine (CoPc) and iron phthalocyanine (FePc) and binuclear (Co-Fe)Pc films by MBE. Binuclear (Co-Fe)Pc films were found to grown only on sapphire substrates at 200^0C if deposited using the CoPc/FePc mixture in 1:1 (w/w) ratio. Formation of binuclear was confirmed by MALDI (Multi Assisted Laser Desorption and Ionization) mass spectroscopy. Binuclear films have better face-on and edge-on overlapping compare to individual CoPc and FePc films. Better face-on stacking was also supported by GIXRD. The in binuclear (Co-Fe)Pc films exhibited μ ~110 cm^2/Vs , which is higher by two orders as compare to CoPc and FePc films. Furthermore temperature dependence of resistivity showed that binuclear films are in metallic regime, while pure films are in the critical regime of metal-insulator transition. These films exhibited trap-free space charge limited conduction (SCLC) in the temperature range 300K to 25K; while pure films showed SCLC with exponential distribution of traps at low temperature. A comparison study of the gas sensing characteristics CoPc, FePc and binuclear (Co-Fe)Pc films has been studied. It has been found that binuclear films are better for gas sensing because of their high mobility.

Charge conduction in FePc films under high electrical field (i.e. upto 20MV/m) has been investigated.

A bias dependent transition from ohmic to space-charge limited conduction to space charge limited conduction with field enhanced mobility is observed. At temperatures <100 K, by analyzing the low bias (< 100 V) data, which is governed by Schottky – barrier limited conduction. However at higher bias multistep tunneling was observed in the FePc films.

A novel feature i.e. temperature dependent metal to insulator like transition, has been observed in ultrathin CoPc films deposited on (001) $SrTiO_3$ substrates. In-plane compressive strains induced by structural phase transition of $SrTiO_3$ substrate reduce the intermolecular distance, and as a result, metallic behavior is observed.

Moreover phthalocyanine based heterojunction comprising of *p*-type CoPc and *n*-type F_{16}CuPc using MBE were fabricated. The *J-V* characteristic of heterojunction shows ohmic conductance with two order of magnitude higher conductivity as compare to individual CoPc and F_{16}CuPc films. The higher conductivity F_{16}CuPc/CoPc hetrojunction is due to the charge carrier accumulation at interface, which is further confirmed by Kelvin probe study.

Gas sensing properties of water soluble copper phthalocyanine (CuTsPc) films prepared by solution process were also studied. These films exhibited room temperature sensitivity towards $C1_2$ gas. Selectivity, repeatability, stability and linearity (sensitivity vs concentration) in the range 5ppb to 2000ppb are investigated.

Publications

In Journals

1. Enhanced Cl2 sensitivity of ultrathin bi-nuclear cobalt-phthalocyanine/ironphthalocyanine films, Arvind Kumar, A. K. Debnath, S. Samanta, A. Singh, R. Prasad, S. Singh, S. Basu, D. K. Aswal, S. K. Gupta, Sensors and Actuators B 171, 423 (2012).

2. Fluorinated copper-phthalocyanine / cobalt-phthalocyaine organic heterojunctions: Charge transport and Kelvin Probe study, A. K. Debnath, Arvind Kumar, S. Samanta, R. Prasad, A. Singh, S. Singh, S. Basu, D. K. Aswal, S. K. Gupta, *Appl. Phys. Lett.* 100, 142104 (2012*).*

3. Metal – semiconductor transition in ultrathin cobalt-phthalocyanine films grown on SrTiO3 single crystal substrates, S. Samanta, Arvind Kumar, A. Singh, A. K. Debnath, S. Basu, R. Prasad, D. K. Aswal, S. K. Gupta and J.V. Yakmi, *Appl. Phys. Lett.* 100, 162101 (2012).

4. Metallic-like conduction in Co-phthalocyanine/Fe-phthalocyanine composite films grown on sapphire substrates, Arvind Kumar, Ajay Singh, S. Samanta, A. K. Debnath, D. K. Aswal, and S. K. Gupta, *Appl. Phys. Lett.* 99, 112102 (2011).

5. Charge transport in ultrathin iron-phthalocyanine thin films under high electric fields, Arvind Kumar, Ajay Singh, Soumen Samanta, K. Vasundhara, A. K. Debnath, D. K. Aswal, S. K. Gupta and J. V. Yakhmi, *J. Phys.: Condens. Matter,* 23, 355801 (2011).

6. Room temperature ppb level Cl2 sensing using sulphonated copper phthalocyanine films Arvind Kumar, Ajay Singh, A.K. Debnath, Soumen Samanta, D.K. Aswal, S.K. Gupta, J.V. Yakhmi, *Talanta,* 82, 1485 (2010).

7. Role of central metal atom and chemisorbed oxygen in gas sensing mechanism for cobalt-phthalocyanine thin films Arvind Kumar, Ajay Singh, A.K. Debnath, Soumen Samanta, D.K. Aswal, S.K. Gupta, *Asian Journal of Physics,* 19, 207 (2010).

In Conference/Symposia

1. Charge transport and Kelvin probe study of organic semiconductor heterojunction, Arvind Kumar, S. Samanta, A. Singh, A. K. Debnath, D. K. Aswal and S.K. Gupta, *AIP Conference Proceedings of TFST(Thin Film: Science and technology), 2011 (to be published).*

2. Trap free space charge limited conduction and high mobility in cobalt phthalocyanine - iron phthalocyanine composite thin films, Arvind Kumar, S. Samanta, Ajay Singh, A. K. Debnath, D. K. Aswal and S.K. Gupta, *Advances of material sciences and technology-2012 Gujarat University, (to be published in Solid State Phenomena).*

3. Reverse rectification behavior in NiPc/F16CuPc heterojucntion, Arvind Kumar, Soumen Samanta, Ajay Singh, A. K. Debnath, D. K. Aswal and S.K. Gupta, *AIP Conference Proceedings 56th DAE solid state physics symposium-2011, SRM university Chennai, 1447, 755 (2012).*

4. Mechanism of charge transport in cobalt and iron phthalocyanine thin films grown by molecular beam epitaxy, Arvind Kumar, Soumen Samanta, Ajay Singh, A. K. Debnath, D. K. Aswal and S.K. Gupta, *AIP Conference Proceedings of International Conference on Advances in Condensed and Nano Materials-2011-Chandigarh,1393, 15 (2011).*

5. Temperature dependent current-voltage characteristics of iron-phthalocyainthine films, A. K. Debnath, A. Kumar, S. Samanta, A. Singh, D. K. Aswal, S. K. Gupta, J. V. Yakhmi*, AIP Conference Proceedings of 55th DAE solid state physics symposium 1349 1047- 1048 (2010).*

6. Electrical and positron study of the interface of organic semiconductor heterojunction, Adrica Kyndiah, Arvind Kumar, S. Samanta, Ajay Singh, A. K. Debnath, J. V. Yakhmi, Priya Maheshwari, and P. K. Pujari, *AIP Conference Proceedings of International Conference on Physics of Emerging Functional Materials (PEFM-2010) 1313, 409-411 (2010).*

Name	:	**Payal Mohanty**
Enrolment No.	:	PHYS04200704006
Constituent Institute	:	Variable Energy Cyclotron Centre, Kolkatta
Title	:	Electromagnetic Radiation from Partons and Hadrons

Abstract

The primary goal of the nuclear collision experiments at ultra-relativistic energies is to create and study a state of matter, the properties of which are governed by the quarks and gluons, such a state of matter is called quark gluon plasma (QGP). Finding out the signals of QGP formation in heavy ion collisions is one of the biggest challenge in the field of high energy nuclear collisions. Electromagnetic probes *i.e.* photons and dileptons are considred to be particularly useful because they are produced during the entire evolution of the system and do not have any final state interactions and hence can carry the information of the source point very effectively.

It is well known that the average magnitude of radial flow at the freeze-out surface can be extracted from the transverse momentum (p_T) spectra of the hadrons. However, hadrons, being strongly interacting objects, can bring the information of the state of the system when it is too dilute to support collectivity; that is, the parameters of collectivity extracted from the hadronic spectra are limited to the evolution stage where the collectivity ceases to exist. These collective parameters have hardly any information about the interior of the matter. In contrast to hadrons, EM radiations are produced and emitted from each space-time point. Therefore, estimating flow from the EM probes will shed light on the time evolution of the collectivity in the system. In the present work it is proposed that photons and dileptons can be used to study the evolution of the collectivity in the QGP phase and hadronic phases which can be used as a signal for the QGP formation.

The radial flow of the QGP and hadronic phases have been estimated by using the ratio of the transverse momentum (p_T) spectra of photons to dileptons. While evaluating the individual photon and dilepton spectra, the initial and freeze-out conditions are constrained by the available experimental data rendering the outcome of the analysis largely model independent.

The Bose-Einstein correlations between dilepton pairs produced in relativistic heavy-ion collisions have been used for the first time in the literature for studying the mass dependence of the HBT (Hanbury-Brown-Twiss) radii. It is shown that the variation of the HBT radii with the invariant mass can be used as a useful tool to characterize the quark-gluon phase. We show that the mass dependence of radii extracted from the virtual photon (dilepton) interferometry provide access to the development of collective flow with time. It is argued that the non-monotonic variation of HBT radii with invariant mass of the lepton pairs signals the formation of quark gluon plasma in heavy ion collisions. The proposal of experimentally measuring the ratio, R_{out}/R_{side} for dileptons can be used to estimate the average life times of the partonic as well as the hadronic phases.

The variation of elliptic flow of thermal dileptons with p_T and invariant mass of the pairs for Pb+Pb collisions at LHC energy has been studied. We find that a judicious selection of M and p_T windows can be used to extract the collective properties of quark matter, hadronic matter and also get a distinct signature of medium effects on vector mesons.

Publications

Refereed Journals:

1. Elliptic Flow of Thermal Dileptons as a Probe of QCD Matter. Payal Mohanty, Victor Roy, Sabyasachi Ghosh, Santosh K. Das, Bedangadas Mohanty, Sourav Sarkar, Jane Alam, Asis K. Chaudhuri. Phys. Rev. C 85 (2012) 031903 (R) Preprint : Nucl-th/1111.2159

2. Evolution of Collectivity as a Signal of Quark Gluon Plasma Formation in Heavy Ion Collisions. Payal Mohanty, Jan-e Alam, Bedangadas Mohanty. Phys. Rev. C 84 (2011) 024903. Preprint : Nucl-th/1008.1112.

3. Characterizing the Partonic Phase by Dilepton Interferometry. Payal Mohanty, Jan-e Alam, Bedangadas Mohanty. Nucl.Phys.A 862 (2011)301-303. Preprint : Nucl-th/1101.4120.

4. Radial Flow from Electromagnetic Probes and Signal of Quark Gluon Plasma. Payal Mohanty, Jajati K Nayak, Jan-e Alam, Satosh K Das. Phys. Rev. C 82 (2010) 034901. Preprint : Nucl-th/0910.4856

5. Nuclear Suppression at Low energy Heavy Ion Collision. Santosh K das, Jan-e Alam, Payal Mohanty, Bikash Sinha. Phys.Rev.C 81 (2010) 044912. Preprint : Nucl-th/0910.4853

6. Dragging Heavy Quarks in Quark Gluon Plasma at the Large Hadron Collider. Santosh K das, Jan-e Alam, Payal Mohanty. Phys. Rev. C 82 (2010) 014908. Preprint : Nucl-th/1003-5508

7. Probing Quark Guon Plasma Properties by Heavy Flavors. Santosh K das, Jan-e Alam, Payal Mohanty. Phys.Rev.C 80 (2009) 054916. Preprint : Nucl-th/0908.4194

Axiv Submission:

1. Thermal Radiation from an Expanding Viscous Medium. Sukanya Mitra,Payal Mohanty, Sourav Sarkar,Jan-e Alam. Preprint : Nucl-th/1107.2500.

Conference Proceedings in Journals:

1. Equilibration in Quark Gluon Plasma. Santosh K das, Jan-e Alam, Payal Mohanty. Indian J. Phys 85 (2011)1149-1153. Preprint : Nucl-th/ 0912.4089.

2. \Scaling Quark Gluon Plasma by HBT Interferometry with Lepton Pairs Payal Mohanty, Jan-e Alam Proceedings of Science PoS(WPCF2011)040 Preprint: Nucl-th/1202.2189

Conference Proceedings:

1. Freeze Out Time in Ultra-Relativistic Heavy Ion Collisions. Santosh K Das, Payal Mohanty, Jajati K Nayak and Jan-e Alam Proceedings of DAE Symp. on Nucl. Phys. (India) 52 (2007) 521

2. Flow from Electromagnetic Radiation Payal Mohanty, Jajati K Nayak, Jan-e Alam, Satosh K Das. Proceedings of DAE Symp. on Nucl. Phys. (India) 55 (2010) 628

3.   Dilepton Interferometry : a Tool to Charecterize Different Phases of Collision in HIC Payal Mohanty, Jan-e Alam, Bedangadas Mohanty Proceedings of DAE Symp. on Nucl. Phys. (India) 55 (2010) 630

4.   Probing Elliptic Flow of QCD Matter by Lepton Pairs Payal Mohanty, Victor Roy, Sabyasachi Ghosh, Santosh K Das, Bedangadas Mohanty, Sourav Sarkar, Jan-e Alam, Asis K Chaudhuri Proceedings of DAE Symp. on Nucl. Phys. (India) 56 (2011) 910

5.   Thermal Radiation from an Expanding Viscous Medium Sukanya Mitra, Payal Mohanty, Sourav Sarkar, Jan-e Alam Proceedings of DAE Symp. on Nucl. Phys. (India) 56 (2011) 936

6.   Dilepton Interferometry at Different Collision Energies Payal Mohanty, Jan-e Alam, Bedangadas Mohanty Proceedings of DAE Symp. on Nucl. Phys. (India) 56 (2011) 960

Name	:	**Shreyashkar Dev Singh**
Enrolment No.	:	PHYS03200704010
Constituent Institute	:	Raja Ramanna Centre for Advanced Technology, Indore
Title	:	MOVPE Growth and Characterization of Quantum Structures Based on III-V Semiconductors

Abstract

InP/GaAs quantum well (QWs) and superlattice structures of high crystalline and interfacial quality have been grown by metal organic vapour phase epitaxy (MOVPE) technique. The issue of type-II band alignment ofr InP/GaAs heterostructure is addressed by means of simple layered architecture of ultrathin quantum wells (QWs). Specific signatures of the radiative recombination in type II QWs, especially, the cube root dependence of the blueshift in the lowest excitonic transition energy on excitation power has been observed in photoluminescence (PL) measurements. This indicates that the observed luminescence originates from spatially separated electrons and holes. The blueshift increases with QW thickness which alos confirms the type-II band alignment. A direct evidence of electron confinement in the conduction band of InP is provided by the capacitance-voltage (C-V) measurements where a well-defined peak in the apparent carrier density (ACD) profile for InP/GaAs ultrathin QWs is observed at low temperatures in the vicinity of QWs. Apart from this, ACD peak value decreases and its width increases with rise in temperature. Additionally, ACD peak value is found to decrease with the QW thickness. These observations confirm that the peak in ACD profile is related to the two dimensional electron-gas occupying the quantum states of ultrathin QWs moreover, ground state (GS) transition energy obtained form PL measurements shifts to lower energy with temperature and it is found that the temperature dependence of the transition energy is similar to the band gap variation of GaAs barrier layer. Furthermore, elastic-relaxation-induced barrier layer thickness fluctuations are observed for InP/GaAs type-II QW superlattice structures. Crystalline and interfacial quality of superlattice structures is reasonable for thick barrier layers of GaAs, and strain is easily accommodated in the GaAs barrier layers, thus confirming the pseudomorphic growth. However, for thin GaAs barrier layers, interfacial and crystalline qualities of the superlattice samples are poor, because the strain between adjacent InP QW is coupled more effectively. It leads to the partial relaxation of the superlattice structures through undulations in GaAs barrier layer thickness. However, study of optical properties of these superlattice structures through photoreflectance (PR) measurements suggests that the built-in electric field in the superlattice structures considerably modifies the temperature dependence of the GS transition energy. For moderate electric fields, the temperature dependence of the GS transition energy follows the bandgap of the GaAs barrier layer, and it decreases at a faster rate than that of the GaAs material in the case of larger values of built-in electric field. In addition to this, signature of optical absorption in the highly strained and partially relaxed superlattice structures is clearly observed at room temperature. Strong coupling effects between the wave functions of confined carriers in the neighbouring qauantum wells on Inp/GaAs type-II superlattice structures are observed in electroreflectance (ER) spectra. (ER) measurements provide clear signatures of the superlattice feature for partially relaxed superlattice stuructures. However, both ER and PR measurements provide the signature of superlattice features for highly strained superlattice structures. Additionally, increase in the surface photovoltage magnitude for energies lower than the band edge position of GaAs buffer layer confirms that the absorption takes place between the electronic minibands formed in the type-II superlattice structures.

Publications

Journals Included in the Thesis

1. Observation of electron confinement in InP/GaAs type-II ultrathin quantum wells. S. D. Singh, V. K. Dixit, S. Porwal, Ravi Kumar, A. K. Srivastava, Tapas Ganguli, T. K. Sharma, and S. M. Oak. Appl. Phys. Lett., 97, 111912 (2010).

2. Temperature dependence of the photoluminescence from InP/GaAs type-II ultrathin quantum wells. S. D. Singh, S. Porwal, K Alexander, V. K. Dixit, A. K. Srivastava, and S. M. Oak. J. Phys. D: Appl. Phys, 43, 455410 (2010).

3. Conduction band offset and quantum states probed by capacitance-voltage measurements for InP/GaAs type-II ultrathin quantum wells. S. D. Singh, V. K. Dixit, Shailesh K. Khamari, Ravi Kumar, A. K. Srivastava, Tapas Ganguli, and S. M. Oak. J. Appl. Phys., 109, 073702 (2011).

4. Effect of built-in electric field on the temperature dependence of transition energy for InP/GaAs type-II superlattices. S. D. Singh, S. Porwal, A. K. Srivastava, T. K. Sharma, and S. M. Oak. J. Appl. Phys., 110, 123523 (2011).

5. Elastic relaxation induced barrier layer thickness undulations in InP/GaAs type-II quantum well superlattice structures. S. D. Singh, Ravi Kumar, C. Mukherjee, Puspen Mondal, A. K. Srivastava, Tapas Ganguli, T. K. Sharma, and S. M. Oak. Semicond. Sci. Technol., 27, 105031 (2012).

6. Signature of optical absorption in highly strained and partially relaxed InP/GaAs type-II quantum well superlattice structures. S. D. Singh, S. Porwal, T. K. Sharma, and S. M. Oak. J. Appl. Phys., 112, 093505 (2012).

Not included in the Thesis

7. Temperature dependence of the lowest excitonic transition for an InAs ultrathin quantum well. S. D. Singh, S. Porwal, T. K. Sharma, and K. C. Rustagi. J. Appl. Phys., 99, 063517 (2006).

8. Spectroscopic investigations of MOVPE-grown InGaAs/GaAs quantum wells with low and high built-in strain. T. K. Sharma, S. D. Singh, S. Porwal, and A. K. Nath J. Crystal Growth, 298, 527 (2007).

9. Comparative study on passivation of $GaAs_{0.86}P_{0.14}/Al_{0.6}Ga_{0.4}As$ near-surface quantum well. Suparna Pal, S. D. Singh, S. W. D'Souza, S. R. Barman, and S. M. Oak. J. Vac. Sci. Technol. A, 28, 1319 (2010).

10. Determination of band offsets in strained $InAs_xP_{1-x}/InP$ quantum well by capacitance voltage profile and photoluminescence spectroscopy. V. K. Dixit, S. D. Singh, S. Porwal, Ravi Kumar, Tapas Ganguli, A. K. Srivastava, and S. M. Oak. J. Appl. Phys., 109, 083702 (2011).

In Edited Proceedings Included in the Thesis

1. Structural, optical and electrical properties of MOVPE grown InP/GaAs type- II ultrathin quantum well. S. D. Singh, V. K. Dixit, S. Porwal, Ravi Kumar, Shailesh K. Khamari, A. K. Srivastava, Tapas Ganguli, and S. M. Oak. International Conference on Physics of Emerging Functional Material (PEFM- 10), BARC, Mumbai, AIP Conf. Proc. 1313, 250 (2010).

2. Quantum states probed by temperature dependence capacitance-voltage measurements for InP/GaAs type-II ultrathin quantum well. S. D. Singh, V. K. Dixit, Shailesh K. Khamari, Tapas Ganguli, and S. M. Oak. DAE-Solid State Physics Symposium, AIP Conf. Proc. 1349, 1109 (2011)

Not included in the Thesis

3. Impact of growth parameters on the structural properties of InP/GaAs type-II quantum dots grown by metal-organic vapour phase epitaxy. S. D. Singh, T. K. Sharma, C. Mukharjee, and S. M. Oak. International Workshop on Physics of Semiconductor Devices, IEEE, 04472543 (2007).

4. tudies on GaAs/AlGaAs based (p and n-type) Quantum Well Infrared Phoxxiv todetector Structures grown using MOVPE. V. K. Dixit, S. D. Singh, T. K. Sharma, Tapas Ganguli, Ravindra Jangir, Suparna Pal, B. Q. Khattak, A. K. Srivastava, Himanshu Srivastava and S. M. Oak. International Workshop on Physics of Semiconductor Devices, IEEE, 04472517 (2007).

5. Blue shift in GaAs0.86P0.14/Al0.6Ga0.4As Near Surface Quantum Well. Suparna Pal, S. D. Singh, S. Porwal, and S. M. Oak. DAE-Solid State Physics Symposium, AIP Conf. Proc. 1349, 1079 (2011).

In Conference Proceedings Included in the Thesis

1. Structural and optical properties of metal organic vapour phase epitaxy grown InP/GaAs type-II ultrathin quantum well. S. D. Singh, V. K. Dixit, S. Porwal, Ravi Kumar, A. K. Srivastava, Tapas Ganguli, and S. M. Oak. DAE-BRNS National Laser Symposium, RRCAT, 2010.

Name   :   **S. V. Desa**
Enrolment No.   :   ENGG01200704026
Constituent Institute   :   Bhabha Atomic Research Centre, Mumbai
Title   :   Analysis of Electromagnetic Welding Process for Thin Similar
                                and Dissimilar Metallic Strips

Abstract

Electromagnetic Welding (EMW) is an impact welding process and hence it is characteristically different than the other conventional fusion welding processes. It offers many distinct advantages, provided it is used, taking into account its limitations. In the field of conventional welding, there are mainly two challenging propositions, namely--- i) welding of aluminium and ii) welding of dissimilar metals. The welding of aluminium is difficult due to its oxidation and welding of dissimilar metals is the cause of concern due to difference in their melting points. The use of aluminium and its alloys, which are light weight metals, is going to increase in future (especially in automobile and aerospace industries). There will be many applications in which welding of aluminium will be required with other metallic parts. Similarly, the welding of metals like copper, Stainless Steel (abbreviated as S.S. hereafter) etc is required for the fabrication of components in various engineering industries. Considering this scenario, the analysis of EMW process for Al, Cu and S.S. with similar and dissimilar combinations, is undertaken in the present work.

In contrast to the aforementioned difficulties, aluminium is the easiest to weld electromagnetically. EMW offers solution to some of the problems mentioned above owing to the fact that the welding is achieved by impact and the melting point and other thermal properties do not of much significant role. The processes like surface preparations, storing in inert atmosphere etc could be eliminated in EMW operation. Apart from this, EMW has many other advantages such as high production rate, reproducibility, automation ease, no need of preparatory methods etc. This warrants serious consideration for harnessing its potential. On the other hand, there are some limitations of the EMW process, which include-1) It is less efficient for metals with low electrical conductivity and 2) It is not suitable for large size jobs (exceeding about 1 meter). The R&D efforts should be focused, taking into consideration the aforementioned advantages and limitations.

Extensive literature survey was undertaken to know the present status of the technology and to decide the course of research to be undertaken. The present research work covers the detailed analysis of welding process for the above metals, based on 5 computational and experimental data. Although the research work under EMF (Electromagnetic Forming) and EMW technologies has been reported for last 25 years, this technology is in its infancy as regards it's commercial adoption. Many aspects of the EMF/EMW technology such as description of the equipment, mathematical modeling of the process, metallurgical/mechanical investigations etc. have been reported in the literature. However, it is found that the R&D efforts are not sufficiently focused from the industrial application point of view. Research papers are available in EMW for tubular geometries. The dependence of electromagnetic parameters on the welding has been studied to a certain extent for tubular job pieces. However, the work on welding of flat strips is reported of lately. In the present work, efforts are concentrated in the analysis of welding process for flat strips. This configuration is chosen considering the limited R & D work on this geometry. Needless to say the analysis procedure could be easily extended for tubular jobs as well. The explosive welding (EXW) also is impact welding process and bonding mechanism is similar in EMW and EXW. The comparison between the two becomes necessary so as to understand their relative merits and demerits. The thesis covers this aspect and underlines the direction of R&D efforts.

The chapter on the 'Introduction' covers the principle of operation, salient features, advantages and limitations of the EMF/EMW processes. The chapter on 'Theoretical and computational analysis' covers the basic theory, design of welding coil, electrical circuit analysis and discussion regarding EMW bonding mechanism and nature of weld interface.

The soft wares like MATLAB SIMULINK, MAXWELL-SV and ANSYS were used for the computational analysis. The computational procedure is formulated (by interfacing the above soft wares) to establish the relationship between electromagnetic and circuit parameters and impact welding force (Lorentz force). MATLAB software was used in estimating the magnitude and shape of current generated by the coil. It was also useful in deciding the coupling factor between the coil and the job piece. This was decided by comparing the computed result with the measured current given by the oscilloscope. MAXWELL-SV software was used for the computation of magnetic field and the Lorentz force. This software was useful in deciding the optimum cross section of the coil. The dependence of parameters like input energy, ringing frequency, coil 6 conductor cross section, job piece material and configuration etc on the Lorentz force is studied with the help of MAXWELL software. ANSYS software was used for the calculation of deformation and collision velocity.

The chapter on 'Computational analysis' discusses the features of the softwares used. It also discusses the procedures followed in handling the softwares. The equations handled and the approximations involved are also discussed. Thus by using these soft wares it was possible to establish the computational procedure for Lorentz force and collision velocity. The computed results were verified by experimental results. The experimental verification of collision velocity was done with measurement of Laser beam intensity.

A 10 kJ, 10 kV facility was set up to carry out the welding experiments. The main components of the welding facility were- the energy storage capacitor bank, high voltage charging power supply, spark gap and it's trigger circuit, field shapers, welding coil (with and without driver), current shunt and storage oscilloscope. These system details are described under the chapter of 'Description of experimental and diagnostic system'.

It may be mentioned that in EMW processes, the two colliding job pieces get electromagnetically deformed before getting welded. Thus, some amount of energy is spent in deformation. In free forming the job piece comes to rest after completion of the deformation process and full kinetic energy is used. However, in EMW process, the energy is partly used in deformation and the remaining kinetic energy is used in impact welding. Hence, some of the conclusions regarding the electrical parameters of the system can be applied to EMF process as well. This fact underlines the versatility and importance of data generated in the present work.

The collision velocity ultimately decides the quality of weld. The literature on EMW also discusses the dependence of collision angle on the weld. However, we have not concentrated on this aspect. The collision velocity is as important as melting point in conventional welding. However, since in the analysis of EMW process, the deformation energy and kinetic energy play important role, the properties like mass density and yield strength have to be considered along with the electrical properties.

The magnitude of collision velocity is decided by Lorentz force and geometrical separation between the coil and job piece. We have decided the lower limit of collision 7 velocity to achieve welding. It is

observed that collision velocity of 400 m/s is required to achieve welding in most of the metals. The input energy required to generate this velocity however, depends on the mechanical and material properties and dimensions of job piece material.

One of the important contributions of this work is the analysis of EMW process by the use of conducting drivers. The drivers are used to improve the performance of welding process in case of low electrical conductivity metals. It is observed that the efficiency of the process can be improved by the use of aluminum drivers. Qualitative information is found in the literature in this regard. With the help of extensive computational and experimental work was undertaken to study the performance of the driver, it can be proved that one can achieve welding in copper and S.S. at lesser energy with aluminium driver, as compared with that achieved without using the latter. Quantitative information about the dimensions of the driver such as thickness and length as a function of ringing frequency is given. Procedure is explained about optimization of the dimensions of the driver. It is shown that aluminium driver with 0.5 mm thickness gives optimum performance at 18 kHz frequency. The performance of the aluminium driver is compared with other drivers (Cu and S.S.). This conclusion is valid for given values of electrical, mechanical and physical properties of the driver material. This type of data is generated and reported for the first time.

We have described a procedure to establish the scaling estimations for capacitive input energies for jobs of different sizes. Data is given for welding of strips of aluminium, copper and S.S. for similar and dissimilar combinations. Aluminium is used as driver to achieve welding for the combinations other than Al-Al. The scaling estimations for input energy are established with the help of verification of computational and experimental results for small size strips. The results are then extrapolated for large size jobs. The collision velocity of 400 m/s is taken as basis for achieving welding. This information can help the designer, to select and standardize the system and process parameters. It may be noted that this data is also reported for the first time.

The welding results were substantiated by mechanical tests and microstructure analysis. The effect of collision velocity and separation distance on the microstructure is discussed to some extent. The thesis also includes discussion on weld interface. Since the 8   main emphasis of the work is focused on 'Electromagnetic analysis', the detailed microstructure analysis falls out of the scope of the present research work.

The important conclusions of the work could be summarized as follows-

1) The feasibility of Electromagnetic welding of similar and dissimilar metal strips is substantiated with quantitative data.

2) A computational model is developed to establish the relationship between electromagnetic and circuit parameters and the impact welding force (Lorentz force)

3) The relationship between Lorentz force and the collision velocity is analyzed. This can help in selection of separation distance between the jobs.

4) Computational procedure is evolved to calculate the collision velocity for a given input energy, by interfacing of computational softwares.

5) It is observed that the collision velocity is the parameter that decides the quality and occurrence of the weld. The thermal properties do not play significant role. However, the mechanical (such as yield strength) and physical (such as mass density) properties play important role in deciding the collision velocity, along with the obvious role of the electrical properties.

6)   It is established that collision velocity of 400 m/s and above is required to achieve welding for most of the metals.

7)   Aluminium proves to be the best driver material to achieve welding in most of the metals.

8)   Scaling estimations for the capacitive input energy is possible for welding of jobs of different materials and sizes, taking 400 m/s as the criterion for achieve welding.

Publications

1.   S. V. Desai, Satendra Kumar, P. Satyamurthy, J. K. Chakravartty and D. P. Chakravarthy 'Analysis of the effect of collision velocity in Electromagnetic Welding of aluminum strips', Int. Journal of Applied Electromagnetics and Mechanics, Vol.34, 2010, pp-131-139.

2.   S. V. Desai, Satendra Kumar, P. Satyamurthy , J.K.Chakravartty and D. P. Chakravarthy, 'Improvement of performance of Electromagnetic welding process by use of driver materials', Int. Journal of Applied Electromagnetics and Mechanics, Vol. 32,2010, pp- 1-9.

3.   S. V. Desai, Satendra Kumar, P. Satyamurthy , J. K. Chakravartty and D. P. Chakravarthy 'Scaling relationships for input energy in Electromagnetic welding of similar and dissimilar metals', Journal of Electromagnetic analysis & Applications Vol. 2, Sept.2010, online- http://www.SciRP.org/journal/jeamaa

Name : **Haridas Pai**
Enrolment No. : PHYS04200704004
Constituent Institute : Variable Energy Cyclotron Centre, Kolkatai
Title : Study of Nuclear Structure Near the Z=82 and N=82 Shell
Closures

Abstract

This thesis work is devoted to the experimental investigation of the high spin structure of the nuclei near Z = 82 and N = 82 shell closures. In the present work, the high spin states in ^{194,197}Tl (Z = 81) and $^{195-198}$Bi (Z = 83) with proton numbers close to and on either side of the Z = 82 spherical shell closure and in ^{134}Cs (Z = 55) with neutron number close to the N = 82 spherical shell closure have been studied by high resolution gamma ray spectroscopic method. Fusion-evaporation reactions, using both heavy and light ion beams, were used to populate the high spin states in these nuclei. Several experiments were performed at three major accelerator centers in India i. e. at VECC (Kolkata), TIFR (Mumbai) and IUAC (New Delhi) and different configurations of the Indian National Gamma Array (INGA), consisted of Clover HPGe detectors, were used in these investigations. A small in-house setup at VECC, consisted of a clover, a single crystal HPGe and a LEPS (Low Energy Photon Spectronmeter) detector was also used for one of the experiments using a beam. New and improved level schemes of these nuclei have been proposed in this work which were obtained from the analysis of *y-y* matrices and *y-y-y* cubes. The coincidence relations among the detected y-rays and their intensity relations were used to build up the level schemes. Definite spin and parity of the excited states in these nuclei were assigned from the knowledge of the multipolarity and type (electric or magnetic) of the emitted y-rays which were determined from the Directional Correlation of Oriented (DCO) states ratio and the Integrated Polarization (IPDCO) measurements, respectively. The Total Routhian Surface (TRS) calculations were performed using cranked shell model with Woods-Saxon potential to understand the results obtained in this work. For the Magnetic Rotational (MR) bands, observed in this work, the particle-hole interaction strengths were determined using semiclassical calculations.

The nuclei near the Z = 82 and the N = 82 shell closures in A ~ 190 and A ~ 130 mass regions, respectively, are crucial laboratories to observe interesting nuclear structure phenomena and to test a variety of nuclear models. The proximity of the spherical shell closures and competing shape (prolate and oblate) driving effects of the high-j orbitals ($\pi h_{9/2}$, $\pi i_{13/2}$ & $v i_{13/2}$ for Thallium and Bismuth nuclei and $\pi h_{11/2}$ & $v h_{11/2}$ for the Cesium nucleus), near the proton and neutron Fermi levels, induce shape co-existence and triaxiality in the nuclei in these regions. Therefore, in both the regions different kinds of excitations are expected.

In the present thesis work, a rotational band in ^{195}Bi has been observed at low excitation which clearly suggests that onset of deformation takes place in the isotopic chain of Bi nuclei at N = 112. In other words, present thesis work indicates that the effect of N = 126 shell closure to reinforce the spherical shape in nuclei lessens for neutron number N ≤ 112.

On the other hand, the hitherto, unknown $\pi i_{13/2}$ level has been discovered in ^{197}Tl. In odd-odd nucleus ^{194}Tl, rotational band, based on $\pi h_{9/2} \otimes v i_{13/2}$ configuration, has been extended the band crossing frequency. The properties of this band have been compared with those in ^{190}Tl and ^{198}Tl, which are reported to have contrasting structures. In ^{198}Tl, this band was interpreted as due to chiral symmetry breaking and a triaxial shape has been proposed while the similar band in ^{190}Tl was interpreted assuming

oblate deformation. Therefore, it was important to know the band structure in the intermediate isotopes. In the present work, the band based on the above configuration in ^{194}Tl show similar behaviour as those in ^{190,198}Tl. It has shown that the signature splitting and the moment of intertia for this band is very similar in all these isotopes. The TRS calculations also suggest oblate deformation for all the three isotopes with similar deformation. Moreover, a MR band has also been observed in ^{194}Tl in this work, based on a six quasiparticle configuration. It may be pointed out that it is for the first time that a MR band has been observed for an odd-proton nucleus below Z = 82 in the Pb-Hg region.

In order to extend the present work for the nuclei near N = 82 shell closure, detailed investigation of the high spin states in ^{134}Cs has been carried out. In the present work, the high spin states have been extended up to an excitation energy of 3.8 MeV and spin of 16$^+$ with the observation of several band structures including a band based on $\pi h_{11/2} \otimes v i_{11/2}$ configuration for the first time in this neutron rich nucleus. The lighter, neutron deficient Cesium isotopes are known to be deformed and the band structure based on the above configuration in the odd-odd isotopes, are reported as, arises due to chiral symmetry breaking with a stable triaxial deformation. A very different structure compared to its lighter isotopes has, however, been observed for the $\pi h_{11/2} \otimes v i_{11/2}$ band in ^{134}Cs has been found to be composed of only M1 transitions with no E2 crossover transitions which indicate its MR nature. Therefore, the chirality seems to breakdown for neutron number N = 79 in Cesium isotopes. The tilted axis cranking (TAC) calculations also suggest a change in structure for ^{134}Cs compared to its immediate odd-odd neighbor ^{132}Cs. A close investigation of the calculated TRS shows that a stable triaxial minimum appeared for the lighter isotopes of Cesium up to N = 77 and the surface becomes very gamma soft for the isotopes with N ≥ 79 I.e. as the neutron number is getting closer to the N = 82 shell closure. The results obtained for ^{134}Cs in this thesis work suggest that N = 77 defines the border of triaxial deformation and chirality in odd-odd Cs isotopes.

Publications

(A) Relevant to the present Thesis

In referred journals :

1. Structural change of the unique-parity πh11=2 $\otimes$ vh11=2 configuration in 134Cs. H. Pai, G. Mukherjee, A. Raghav, R. Palit, C. Bhattacharya, S. Chanda, T. Bhattacharjee, S. Bhattacharyya, S.K. Basu, A. Goswami, P.K. Joshi, B.S. Naidu, Sushil K. Sharma, A.Y. Deo, Z. Naik, R.K. Bhowmik, S. Muralithar, R.P. Singh, S. Kumar, S. Sihotra, and D. Mehta. Phys. Rev. C 84, 041301(R) (2011).

2. High spin band structures in doubly-odd 194Tl. H. Pai, G. Mukherjee, S. Bhattacharyya, M.R. Gohil, T. Bhattacharjee, C. Bhattacharya, R. Palit, S. Saha, J. Sethi, T. Trivedi, Shital Thakur, B.S. Naidu, S.K. Jadav, R. Donthi, A. Goswami and S. Chanda. Phys. Rev. C 85, 064313 (2012).

3. Onset of deformation at N = 112 in Bi nuclei. H. Pai, G. Mukherjee, R. Raut, S.K. Basu, A. Goswami, S. Chanda, T. Bhattacharjee, S. Bhattacharyya, C. Bhattacharya, S. Bhattacharya, S.R. Banerjee, S. Kundu, K. Banerjee, A. Dey, T.K. Rana, J.K. Meena, D. Gupta, S. Mukhopadhyay, Srijit Bhattacharya, Sudeb Bhattacharya, S. Ganguly, R. Kshetri, and M.K. Pradhan. Phys. Rev. C 85, 064317 (2012).

Results Reported in Conferences/Symposia :

1. High spin spectroscopy of 134Cs. H. Pai, G. Mukherjee, S. Bhattacharyya, T. Bhattacharjee, R. palit A. Y. Deo, P.K. Joshi, B. S .Naidu, S. Sharma, A. Raghav, Z. Naik, A. Goswami, S. kumar,

S.Sihotra and D. Mehta. Proceedings of the International Symposium on nuclear physics, DAE, Vol 54 88 (2009).

2. Deformed shapes in odd-odd nuclei near Z = 82. G. Mukherjee, H. Pai, S. Bhattacharya, C. Bhattacharya, S. Bhattacharyya, S. Chanda, T. Bhattacharjee, S. K. Basu, S. Kundu, T. K. Ghosh, K. Banerjee, T. K. Rana, J. K. Meena, R. K. Bhowmik, R. P. Sing, S. Muralithar and R. Garg. Proceedings of the International Symposium on nuclear physics, DAE, Vol 54 98 (2009).

3. Structure of Odd-Odd Nucleus 134Cs at High Spin. H. Pai, G. Mukherjee, R.K. Bhowmik, S. Bhattacharyya, T. Bhattacharjee, C. Bhattacharya, S.K. Basu, R. Palit, S. Chanda, A.Y. Deo, P.K. Joshi, B. S. Naidu, Z. Naik, Sushil K. Sharma, A. Raghav, A. Goswami, S. Kumar, S. Sihotra, D. Mehta, S. Muralithar, R.P. Singh, N.S. Pattabiraman and S.S. Ghugre. Nuclear Structure 2010 Clark-Kerr Campus, U. C. Berkeley, CA August 8th – August 13th, 2010.

4. Study of magnetic rotation in 198Bi. H. Pai, G. Mukherjee, S. Bhattacharya,C. Bhattacharya, S. Bhattacharyya, S. Chanda, T. Bhattacharjee, S.K. Basu, S. Kundu, T.K. Ghosh, K. Banerjee, T.K. Rana, J.K. Meena, R.K. Bhowmik, R.P. Singh, S. Muralithar and R. Garg. Proceedings of the DAE Symposium on nuclear physics, Vol 55 80 (2010).

5. Change over from Chiral to Shears geometry in Cs isotopes. G. Mukherjee and H. Pai. Proceedings of the DAE Symposium on nuclear physics, Vol 55 82 (2010).

6. Coexistence of different band structures in odd-odd 194Tl. H. Pai, G. Mukherjee, S. Bhattacharyya, M.R. Gohil, C. Bhattacharya, R. Palit, A. Goswami, T. Bhattacharjee, S. Saha, J. Sethi, T. Trivedi, S. Thakur, B.S. Naidu, S.K. Jadav and R Donthi. Proceedings of the DAE Symposium on nuclear physics Vol 56 198 (2011).

7. Gamma ray spectroscopy of 197Tl using α beam. H. Pai, G Mukherjee, S. Bhattacharyya, M.R. Gohil, C. Bhattacharya, S. Bhattacharya, A. Goswami, T. Bhattacharjee, S. Chanda, K. Banerjee, S.R. Banerjee, A. Chowdhury, P. Chowdhury,T.K. Ghosh, S. Kundu, J.K. Meena, P. Mukhopadhyay, S. Mukhopadhyay, S. Pal, R. Pandey, D. Pandit, G. Prajapati, S. Rajbangshi and T.K. Rana. Proceedings of the DAE Symposium on nuclear physics Vol 56 286 (2011).

(B) Other publications (in refereed journals)

1. Cluster emission in 13C + 12C and 12C + 12C reactions at ~ 6 MeV/Nucleon. T. K. Rana, C. Bhattacharya, S. Kundu, K. Banerjee, S. Bhattacharya, G. Mukherjee, T. K. Ghosh, J. K. Meena, P. Dhara, M. Biswas, H. Pai, K. Mahata, Suresh Kumar, K. Ramachandran, P. C. Rout, S. K. Pandit, V. Nanal and R. G. Pillay. International Journal of Modern Physics E 20, 789 (2011).

2. Measurement and simulation of neutron response function of organic liquid scintillator detector. M. Gohil, K. Banerjee, S. Bhattacharya, C. Bhattacharya, S. Kundu, T.K. Rana, G. Mukherjee, J.K. Meena, R. Pandey, H. Pai, T.K. Ghosh, A. Dey, S. Mukhopadhyay, D. Pandit, S. Pal, S.R. Banerjee and T. Bandhopadhyay. Nucl. Instrum. Meth. Phys. Res. A 664, 304 (2012).

3. Measurement of giant dipole resonance width at low temperature: A new experimental perspective. S. Mukhopadhyay, Deepak Pandit, Surajit Pal, Srijit Bhattacharya, A. De, S. Bhattacharya, C. Bhattacharya, K. Banerjee, S. Kundu, T.K. Rana, G. Mukherjee, R. Pandey, M. Gohil, H. Pai, J.K. Meena and S.R. Banerjee. Physics Letters B 709, 9 (2012).

4. Complex-fragment emission in low-energy light-ion reactions. S. Kundu, C. Bhattacharya, K. Banerjee, T. K. Rana, S. Bhattacharya, A. Dey, T. K. Ghosh, G. Mukherjee, J. K. Meena, P. Mali, S. Mukhopadhyay, D. Pandit, H. Pai, S. R. Banerjee, and D. Gupta P. Banerjee, Suresh Kumar, A. Shrivastava, A. Chatterjee, K. Ramachandran, K. Mahata, S. Pandit and S. Santra. Phys. Rev. C 85, 064607 (2012).

5. Variation of nuclear level density with angular momentum. K. Banerjee, S. Bhattacharya, C. Bhattacharya, M. Gohil, S. Kundu, T. K. Rana, G. Mukherjee, R. Pandey, P. Roy, H. Pai, A. Dey, T.

K. Ghosh, J. K. Meena, S. Mukhopadhyay, D. Pandit, S. Pal and S. R. Banerjee. Phys. Rev. C 85, 064310 (2012).

Results Reported in Conferences/Symposia :

1. Lifetime measurements in 139Pr. S. Chanda, T. Bhattacharjee, S. Bhattacharyya, H. Pai, G. Mukherjee, S. K. Basu, R. Garg, J. Kaur, G. Mohanty, P. Sugathan, R. P. Sing, S. Muralithar, N. Madhavan, A. Jhingan, A. Dhal, R. K. Bhowmik, C. M. Petrache, I. Ragnarsson, S. Bhowal and G. Gangopadhyay. Proceedings of the International Symposium on nuclear physics, DAE, Vol 54 94 (2009).

2. Spectroscopy of 207Rn across isomeric state. S. Bhattacharyya, T. Bhattacharjee, S. Chanda, H. Pai, G. Mukherjee, S. K. Basu, R. K. Bhowmik, A. Dhal, R. Garg, A. Jhingan, J. Kaur, N. Madhavan, G. Mohanty, S. Muralithar, R. P. Sing and P. Sugathan. Proceedings of the International Symposium on nuclear physics, DAE, Vol 54 100 (2009).

3. Isoscaling in 13C + 12C and 12C + 12C reactions at ~ 6 MeV/u. T. K. Rana, C. Bhattacharya, S. Kundu, K. Banerjee, S. Bhattacharya, G. Mukherjee, T. K. Ghosh, J. K. Meena, P. Dhara, M. Biswas, H. Pai, K. Mahata, Suresh Kumar, K. Ramachandran, P. C. Rout, S. K. Pandit, V. Nanal and R. G. Pillay. Proceedings of the International Symposium on nuclear physics, DAE, Vol 54 388 (2009).

4. Measurement of lifetime and transition moments near doubly closed 146Gd. T. Bhattacharjee, D. Banerjee, A. Chowdhury, S. Bhattacharyya, R. Guin, S. K. Das, S. K. Basu, P. Das, C. C. Dey, H. Pai and P. Mukhopadhyay. Proceedings of the DAE Symposium on nuclear physics, Vol 55 12 (2010).

5. Rotational particle coupling in 134Cs. T. Bhattacharjee, H. Pai and S. Bhattacharya. Proceedings of the DAE Symposium on nuclear physics, Vol 55 62 (2010).

6. High Spin Spectroscopy of odd-odd 140Pr. T. Bhattacharjee, S. Chanda, S. Bhattacharyya, H. Pai, G. Mukherjee, S. K. Basu, R. K. Bhowmik, A. Dhal, R. Garg, A. Jhingan, J. Kaur, N. Madhavan, G. Mohanty, S. Muralithar, R. P. Singh and P. Sugathan. Proceedings of the DAE Symposium on nuclear physics, Vol 55 70 (2010).

7. Study of odd Osmium isotopes from EC decay. S. Bhattacharyya, T. Bhattacharjee, D. Banerjee, R. Guin, S. K. Das, H. Pai, A. Chowdhury, G. Mukherjee and P. Das. Proceedings of the DAE Symposium on nuclear physics, Vol 55 78 (2010).

8. Three α-decays of Hoyle state of 12C in 12C + 12C reaction. T. K. Rana, C. Bhattacharya, S. Kundu, K. Banerjee, S. Bhattacharya, G. Mukherjee, T. K. Ghosh, J. K. Meena, P. Dhara, M. Biswas, H. Pai, K. Mahata, Suresh Kumar, K. Ramachandran, P. C. Rout, S. K. Pandit, V. Nanal and R. G. Pillay. Proceedings of the DAE Symposium on nuclear physics, Vol 55 230 (2010).

9. Angular momentum gated neutron evaporation studies. K. Banerjee, S. Kundu, T. K. Rana, C. Bhattacharya, G. Mukherjee, M. Gohil, J. K. Meena, R. Pandey, H. Pai, A. Dey, M. Biswas, S. Mukhopadhyay, D. Pandit, S. Pal, S. R. Banerjee, T. Bandhopadhyay and S. Bhattacharya. Proceedings of the DAE Symposium on nuclear physics, Vol 55 324 (2010).

10. Geant4 simulation of pulse-height response function of liquid scintillator based neutron detector. M. Gohil, K. Banerjee, C. Bhattacharya, S. Kundu, T. K. Rana, G. Mukherjee, J. K. Meena, R. Pandey, H. Pai, M. Biswas, A. Dey, T. Bandhopadhyay and S. Bhattacharya. Proceedings of the DAE Symposium on nuclear physics, Vol 55 720 (2010).

11. Spectroscopy of heavy isotopes of Hg and Au from incomplete fusion reaction. S. Bhattacharyya, S. Dasgupta, H. Pai, A. Shrivastava, G. Mukherjee, R. Palit, T. Bhattacharjee, S. Chanda, A. Chatterjee, V. Nanal, S.K. Pandit, S. Saha and S. Thakur. Proceedings of the DAE Symposium on nuclear physics Vol 56 354 (2011).

12. High spin structure of 200;201Tl isotopes. S. Dasgupta, S. Bhattacharyya, H. Pai, A. Shrivastava, G. Mukherjee, R. Palit, T. Bhattacharjee, S. Chanda, A. Chatterjee, V. Nanal, S.K. Pandit, S. Saha and S. Thakur. Proceedings of the DAE Symposium on nuclear physics Vol 56 356 (2011).

13. Excited states of neutron rich 150Pm using (p, nγ) reaction. T. Bhattacharjee, D. Banerjee, K. Banerjee, S. R. Banerjee, S. K. Basu, C. Bhattacharya, S. Bhattacharya, S. Bhattacharyya, S. Chanda, A. Chowdhury, S. K. Das, T. K. Ghosh, A. Goswami, M. R. Gohil, R. Guin, S Kundu, J. K.

14. Meena, G. Mukherjee, P. Mukhopadhyay, S. Mukhopadhyay, H. Pai, S. Pal, R. Pandey, D. Pandit, G. Prajapati, S. Rajbanshi and T. Rana. Proceedings of the DAE Symposium on nuclear physics Vol 56 358 (2011).

15. Complete spectroscopy of 146Eu using alpha beam from VEC. T. Bhattacharjee, D. Banerjee, P. Das, S. Das, A. Chowdhury, S. Bhattacharyya, R. Guin, H. Pai and P. Mukhopadhyay. Proceedings of the DAE Symposium on nuclear physics Vol 56 372 (2011).

16. Polarization Asymmetry Measurements for the Yrast Band of 85Rb. S. Kumar ,V. Kumar, Ritika. Garg, Naveen. Kumar, S. Verma, S. Mandal,T . Trivedi, S. Saha, J. Sethi, Gayatri, Arindam. Nandi, B.S. Naidu, S.K. Jadav, Rajneesh, R. Palit, D. Choudhary, A.k. Jain, Haridas Pai and G. Mukherjee. Proceedings of the DAE Symposium on nuclear physics Vol 56 322 (2011).

17. Negative Parity States in 86Sr. S. Kumar ,V. Kumar, Ritika. Garg, Naveen. Kumar, S. Verma, S. Mandal,T . Trivedi, S. Saha, J. Sethi, Gayatri, Arindam. Nandi, B.S. Naidu, S.K. Jadav, Rajneesh, R. Palit, D. Choudhary, A.k. Jain, Haridas Pai and G. Mukherjee. Proceedings of the DAE Symposium on nuclear physics Vol 56 400 (2011).

18. Measurement of relative production cross-section of 3n and 4n evaporation channels of an α-induced fusion reaction. Mahua Chakraborty, H. Pai and G. Mukherjee. Proceedings of the DAE Symposium on nuclear physics Vol 56 666 (2011).

19. Extraction of angular momentum gated nuclear level density parameter. K. Banerjee, C. Bhattacharya, M. Gohil, S. Kundu, T. K. Rana, G. Mukherjee, R. Pandey, H. Pai, Pratap Roy, T. K. Ghosh, J. K. Meena, S. Mukhopadhyay, D. Pandit, S. Pal, S. R. Banerjee and S. Bhattacharya. Proceedings of the DAE Symposium on nuclear physics Vol 56 594 (2011).

20. Study of light-particle evaporation spectra (n, p, α) in 4He + 93Nb reaction. Pratap. Roy, K. Banerjee, S. Kundu, T.K. Rana, C. Bhattacharya, M. Gohil, G. Mukherjee, J.K. Meena, R. Pandey, H. Pai, A. Dey, T.K. Ghosh, S. Mukhopadhyay, D. Pandit, S. Pal, S.R. Banerjee and S. Bhattacharya. Proceedings of the DAE Symposium on nuclear physics Vol 56 540 (2011).

21. Structure and decay mechanism of Hoyle state. T. K. Rana, S. Bhattacharya, C. Bhattacharya, S. Kundu, K. Banerjee, G. Mukherjee, J. K. Meena, R. Pandey, M. Gohil, H. Pai, A. Dey, T. K. Ghosh, M. Biswas and G. Prajapati. Proceedings of the DAE Symposium on nuclear physics Vol 56 492 (2011).

22. Study of Single nucleon transfer in α + 12C reaction. R. Pandey, T.K Rana, M. Biswas, A. Dey, C. Bhattacharya, S. Kundu, K. Banerjee, G. Mukherjee, T.K. Ghosh, J.K Meena, H Pai, M Gohil and S Bhattacharya. Proceedings of the DAE Symposium on nuclear physics Vol 56 634 (2011).

23. Low energy neutron response function of BC501A detector. M. Gohil, K. Banerjee, C. Bhattacharya, S. Kundu, T. K. Rana, G. Mukherjee, R. Pandey, H. Pai, P. Roy, T. K. Ghosh, J. K. Meena and S. Bhattacharya. Proceedings of the DAE Symposium on nuclear physics Vol 56 1046 (2011).

Name	:	**Lipika Rani Bairi**
Enrolment No.	:	CHEM02200704001
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam i
Title	:	Development and Characterization of D9 Stainless Steel-Zirconium Metal Waste from Alloys

Abstract

Metal waste form (MWF) is the product of metallic waste generated at the end of pyrochemical reprocessing of spent metallic fuels of fast breeder reactors. It consists of stainless steel (SS) cladding, noble metal fission products (NMFP), contaminated actinides (mainly U) and zirconium from the alloy fuel. This MWF alloys requires to be melted and packing as engineered barrier system forits safe disposal in geological repository. The role of Zr in the alloy is to lower the melting point with the formation of intermetallic phases which act as sink for actinide and fission product elements. Zr-rich intermetallic phases will resist the leaching of radionuclides and prevent ground water contamination. The aim and objectives of this thesis work is to develop highly corrosion resistant metal waste from alloys by optimizing their composition, characterize the phase formed and evaluating their functioning in simulated geological condition. Since, alloy D9 SS is one of the candidate clad materials for the fuel and in the present work D9 SS-Zr MWF alloys were developed by optimizing Zr content. The microstructure, hardness and phase were analysed with emphasis on the assessment of their degradation mechanisms in the simulated geological repository with respect to corrosion, selective elemental leaching and microbiological induced degradation. These studies were extended to D9SS-Zr-NMFP and D9SS-Zr-NMFP-U MWF alloys for the purpose of understanding their leaching behavior of NMFP and U form the MWF alloy phases.

The microstructure of the alloys showed two different types of phases, a dark phase in which the composition was nearly the same as D9 SS alloy and a bright phase comprising Fe-Zr and Ni-Zr type Laves intermetallics. MWF alloys of D9 SS with 8 – 12 wt% Zr showed appreciable corrosion resistance with stable passive film formation in the different simulated geological media. These alloys could accommodate the NMFP and U in the Laves intermetallic phases without any significant corrosion and selective leaching of its alloying elements. Zirconium present in the MWF alloys also formed stable and adherent ZrO_2 layer along with Cr_2O_3 film and protect the alloys from localized attack as well as from breakdown of passive film and selective elemental leaching. However, the bacterial species present in the geological media c n cause microbiologically induced corrosion due to biocompatible nature of Zr.

Publications

In Journals

1. Lipika Rani Bairi, S. Ningshen, U. Kamachi Mudali and Baldev Raj, Microstructural analysis and corrosion behaviour of D9 stainless steel - zirconium metal waste form alloys, Corrosion Science 52 (2010) 2291-2302.

2. Lipika Rani Bairi, S. Ningshen, U. Kamachi Mudali and Baldev Raj, Corrosion issues related to disposal of 316SS-zirconium metal waste form under simulated repository conditions, Corrosion Engineering Science and Technology 46 (2011) 171-176.

3. Lipika Rani Bairi, S. Ningshen, U. Kamachi Mudali and Baldev Raj, Corrosion investigations on metal waste form of titanium modified 316 stainless steel zirconium alloys in simulated ground water medium, Corrosion 68 (2012) 784-792.

4. Lipika Rani Bairi, G. Pannerselvam and U. Kamachi Mudali, High temperature phase stability and microstructural characterization of D9 stainless steel – zirconium metal waste form alloy, Transaction of Indian Institute of Metal 65 (2012) 333-341.

5. Lipika Rani Bairi, R.P. George and U. Kamachi Mudali, Microbially induced corrosion of D9 stainless steel- zirconium metal waste form alloy under simulated geological repository environment, Corrosion Science 61 (2012) 19-27.

6. Lipika Rani Bairi, Bhuvaneswari Gopal, S. Ningshen and U. Kamachi Mudali, Dynamic and static leachability studies and surface characterization of metal waste form alloys for geological disposal Applied Surface Science (under review).

7. Lipika Rani Bairi, C Mallika and U. Kamachi Mudali, Influence of noble metal fission product and actinide on the microstructural and corrosion behaviour of D9 SS-Zr metal waste form alloy, Journal of Nuclear Materials (Communicated)

8. Lipika Rani Bairi, C. Mallika and U. Kamachi Mudali, Distribution of noble metal fission product and its influence in corrosion behavior metal waste form alloy, Corrosion (Communicated)

Conference Proceedings and Oral Presentations

1. Lipika Rani Bairi, S. Ningshen and U. Kamachi Mudali, Electrochemical investigation to evaluate the corrosion behaviour of stainless steel –zirconium metal waste form alloys, Presented in the '14th Natl. Convention of Electrochemists (NCE-14)', IGCAR, Kalpakkam, Dec. (2007).

2. Lipika Rani Bairi, S. Ningshen and U. Kamachi Mudali, Corrosion investigation on Ti modified 316SS- Zr metal waste form alloys in simulated ground water medium, Natl. Symp. 'Electrochemical Science and Technology (NSEST-2009)', Bangalore, India, July (2009).

3. Lipika Rani Bairi, Judy Gopal, S. Ningshen and U. Kamachi Mudali, Characterization of passive films on metal waste form alloys of D9 stainless steel containing zirconium, Internatl. Conf. on 'Surface Modification Technologies (SMT-23)', Mamallapuram, Nov. (2009).

4. Lipika Rani Bairi, S. Ningshen, U. Kamachi Mudali and Baldev Raj, Corrosion issues related to disposal of 316SS - Zr metal waste forms under simulated repository conditions, 4th Internatl. Workshop on 'Long Term Prediction of Corrosion Damage in Nuclear Waste System (Long TermCor2010)', Bruges, Belgium, June - July (2010).

5. Lipika Rani Bairi, Rani P. George and U. Kamachi Mudali, Electrochemical corrosion studies on metal waste form exposed to microbial environments, Chemistry Research Scholar Meet (CRSM-2011), IGCAR, Kalpakkam, July (2011).

6. Lipika Rani Bairi, G. Panneerselvam and U. Kamachi Mudali, High temperature microstructure characterization of D9 stainless steel - zirconium metal waste form alloys, 'Natl. Metallurgist Day - Annual Technical Meeting (NMD-ATM-2011)', Hyderabad, Nov. (2011).

III. Book Chapter

1. Lipika Rani Bairi, Judy Gopal, S. Ningshen and U. Kamachi Mudali, in: T.S. Sudarshan, U. Kamachi Mudali and Baldev Raj (Eds.), Characterization of Passive Films on Metal Waste Form Alloys of D9 Stainless Steel Containing Zirconium, Surface Modification Technology, First ed., Vol. 23, Valardocs, India (2010) pp. 529-536.

IV. Internal Report

1. IGC annual report, 2008, Development of Metal Waste Forms and their Characterization for Microstructure and Corrosion Behaviour, (Article No. IV B 3.2, pp. 154-155)

V. Award and Recognition

1. Best paper award for the paper "Corrosion issues related to disposal of 316SSzirconiumm metal waste form under simulated repository conditions" by Lipika Rani Bairi, S. Ningshen, U. Kamachi Mudali and Baldev Raj in Corros. Engg. Sci. Technol., 46 (2011) 171-176" from Indian Institute of Metal, Kalpakkam Chapter, May 4, 2012.

2. The AFM image of MWF alloys has been recognised as the cover page image in the book of "Surface Modification Technology", Vol. 23, Valardocs, India (2010).

Name   :   **Chitrasen Jena**
Enrolment No.   :   PHYS07200604030
Constituent Institute   :   Institute of Physics, Bhubaneswar i
Title   :   Partticle Production and Elliptic Flow of Light Nuclei in
                                    Relativistic Heavy Ion Collisions at RHIC

Abstract

The theory of strong interactions, Quantum Chromodynamics (QCD), predicts the existence of the new state of matter called Quark-Gluon Plasma (QGP) at sufficiently high temperature and/or high energy density. The experimental program at the Relativistic Heavy Ion Collider (RHIC) is primarily designed to produce and study such a new state of matter. Several measurements taken at RHIC lead to a strong circumstantial evidence for the formation of QGP. Elliptic flow of identified particules is an important observable used towards establishing the formation of partonic matter in the initial stages of the collisions. In this thesis we present the results on elliptic flow of light nuclei in Au+Au collisions at $\sqrt{s_{NN}}$= 39 and 200 GeV measured at mid-rapidity in STAR experiment at RHIC. The measured v_2 for *d(d)* and *^{3}He(^{3}He)* as a function of transverse momentum p_T is found to follow an approximate atomic mass number (A) scaling. The v_2 values for light nuclei are scaled to the number of constituent quarks (NCQ) of their constituent nucleons and are consistent with NCQ scaled v_2 for baryons and mesons. This indicates that partonic collectivity dominates the expansion dynamics of the nucleus-nucleus collisions of RHIC. We have studied the centrality dependence of v_2 for light nuclei and compared those with other hadrons in Au+Au collisions at $\sqrt{s_{NN}}$= 200 GeV. Similar to other hadrons, an increase of p_T-integrated v_2 scaled by the participant eccentricity as a function of collision centrality has been observed, which indicates a stronger collective expansion for more central collision. The mass dependence of average transverse momentum *(p_T)* and the average v_2 have been studied and compared to Tsallis Blast- Wave (TBW) modelpredictions. Both v_2 and *(p_T)* trends are consistent with expectations from TBW model fit. The v_2 of light nuclei measured in Au+Au collisions at $\sqrt{s_{NN}}$= 200 GeV are in good agreement with the dynamical coalescence model calculation. In pursuit of a detailed study of nuclei production in high energy heavy-ion collisions, we have observed for the first time the antimatter helium-4 nucleus *(^{4}He)*, also known as the anti-α in the STAR experiment at RHIC. In total 18 *^{4}He* counts were detected at the STAR experiment in 10^9 recorded Au+Au collisions at $\sqrt{s_{NN}}$= 200 GeV and 62 GeV. The observed *^{4}He* yield is consistent with expectations from thermodynamic and coalescent nucleosynthesis models. This provides an indication of the production rate ofantimatter nuclei through nuclear interactionsand a point of reference for possible future observations in cosmic radiation. This thesis presents the details related to the two *^{4}He* candidates found in the Au+Au collision at $\sqrt{s_{NN}}$= 200 GeV data setcollected in the year 2007. In order to study the QGP, it is also very important to understand the basic nucleon-nucleon interactions and nucleon-nucleus interactions. At RHIC, the measurement of identified particle spectra in *d*+Au collisions would be helpful to understand the initial Cold Nuclear Matter (CNM) effects such as Cronin effect, shadowing and gluon saturation. The Cronin effect, the enhancement of hadron yields at intermediate p_T in *p*+A collisions as compared to those in *p+p* collisions, has received renewed interest at RHIC.In order to understand the particle species dependence of Cronin effect and shed light on the initial conditions at RHIC, we have studied the nuclear modification factor R_{dAu} of the ϕ meson along with π, K and *p* in central *d*+Au collisions at $\sqrt{s_{NN}}$= 200 GeV. The measured R_{dAu} of ϕ meson increases above unity and is higher than R_{AuAu} at intermediate p_T. The enhancement of R_{dAu} of ϕ meson at the intermediate p_T is attributed to be due to the Cronin effect. When we compare of R_{dAu} of ϕ meson with that of other hadrons, it seems to follow othr mesons for 2.5 < p_T< 4GeV/*c.* This result favors the

coalescence as the mechanism for the mid-rapidity particle production in most central *d*+Au collisions. In order to understand the particle production mechanism in forward (deuteron going side) and backward (gold going side) rapidity, we have studied the rapidity asymmetry (Y $_{Asym}$) of ϕ meson is greater than unity in the measured p_T region for both IyI < 0.5 and 0.5 < IyI < 1. Similar to other hadrons, the Y_{Asym} for ϕ meson is found to be larger for 0.5 < IyI < 1 than for IyI < 0.5. This may indicate the presence of some rapidity dependence of nuclear effects. There is no strong particle type dependence observed for Y $_{Asym}$ in the measured pr region.

Publications

1. * Yield and elliptic flow of d(d) and 3He(3He) in Au+Au collisions at √sNN = 200 GeV, Intended for Phys. Rev. C, is under PWG review.
2. * Observation of the antimatter helium-4 nucleus, H. Agakishiev et al. (STAR Collaboration), Nature 473, 353, 2011.
3. * Elliptic flow of light nuclei in Au+Au collisions at √sNN = 200 GeV, C. Jena (for the STAR collaboration), Nucl. Phy. A 862-863, 281 (2011).
4. Longitudinal scaling of observables in heavy ion collision models, Md. Nasim, C. Jena, L. Kumar, P. K. Netrakanti, B. Mohanty, Phys. Rev. C 83, 054902, 2011.
5. * Elliptic flow of light nuclei in heavy ion collisions at STAR, C. Jena (for the STAR collaboration), To be published in Central European Journal of Physics.
6. Inclusive charged hadron elliptic flow in Au+Au collisions at √sNN = 7.7 - 39 GeV, L. Adamczyk et al. (STAR Collaboration), arXiv:1206.5528 [nucl-ex].
7. Di-electron spectrum at mid-rapidity in p+p collisions at √sNN = 200 GeV, L. Adamczyk et al. (STAR Collaboration), arXiv:1204.1890 [nucl-ex].
8. Directed flow of identified particles in Au+Au Collisions at √sNN = 200 GeV at RHIC, L. Adamczyk et al. (STAR Collaboration), Phys. Rev. Lett. 108, 202301 (2012).
9. Identified hadron compositions in p + p and Au+Au collisions at high transverse momenta at √sNN = 200 GeV, G. Agakishiev et al. (STAR Collaboration), Phys. Rev. Lett. 108, 072302 (2012).
10. Directed and elliptic flow of charged particles in Cu+Cu collisions at √sNN = 22.4 GeV, G. Agakishiev et al. (STAR Collaboration), Phys. Rev. C 85, 014901 (2012).
11. Strangeness Enhancement in Cu+Cu and Au+Au Collisions at √sNN = 200 GeV, G. Agakishiev et al. (STAR Collaboration), Phys. Rev. Lett. 108, 072301 (2012).
12. Energy and system-size dependence of two- and four-particle v2 measurements in heavy ion collisions at RHIC and their implications on flow fluctuations and nonflow, G. Agakishiev et al. (STAR Collaboration), arXiv:1111.5637 [nucl-ex].
13. Strange and Multi-strange Particle Production in Au+Au Collisions at √sNN = 62.4 GeV, M.M. Aggarwal et al. (STAR Collaboration), Phys. Rev. C 83, 024901 (2011).
14. Scaling properties at freeze-out in relativistic heavy ion collisions, M.M. Aggarwal et al. (STAR Collaboration), Phys. Rev. C 83, 034910 (2011).
15. An Experimental Exploration of the QCD Phase Diagram: The Search for the Critical Point and the Onset of De-confinement, M.M. Aggarwal et al. (STAR Collaboration), arXiv:1007.2613 [nucl-ex].
16. K_0 production in Cu+Cu and Au+Au collisions at √sNN= 62.4 GeV and 200 GeV, M.M. Aggarwal et al. (STAR Collaboration), Phys. Rev. C 84, 034909 (2011).
17. Charged and strange hadron elliptic flow in Cu+Cu collisions at √sNN = 62.4 and 200 GeV, B.I. Abelev et al. (STAR Collaboration), Phys. Rev. C 81, 044902 (2010).
18. Spectra of identified high-pT π± and p($\bar{\text{p}}$) in Cu+Cu collisions at √sNN = 200 GeV, B.I. Abelev et al. (STAR Collaboration), Phys. Rev. C 81, 054907 (2010).
19. Observation of an Antimatter Hypernucleus, B.I. Abelev et al. (STAR Collaboration), Science 328, 58 (2010).

20. Identified particle production, azimuthal anisotropy, and interferometry measurements in Au+Au collisions at √sNN = 9.2 GeV, B.I. Abelev et al. (STAR Collaboration), Phys. Rev. C 81, 024911 (2010).

21. Center of mass energy and system-size dependence of photon production at forward rapidity at RHIC, B.I. Abelev et al. (STAR Collaboration), Nucl. Phys. A 832, 134 (2010).

22. * Particle production and elliptic flow of light nuclei in relativistic heavy ion collisions at RHIC , C. Jena (for the STAR collaboration), Proceedings for DAE Symposium on Nuclear Physics, Vol. 56, 1180 (2011).

23. * Recent results on identified particle spectra from d+Au collisions at RHIC, C. Jena (for the STAR collaboration), Proceedings for DAE Symposium on Nuclear Physics, Vol. 55, 572 (2010).

24. Simulation framework for Photon Multiplicity Detector in ALICE, C. Jena et al., Proceedings for DAE-BRNS Symposium on Nuclear Physics, Vol. 52, 543 (2007).

25. Status of Photon Multiplicity Detector in ALICE, S.K. Prasad et al., Proceedings for DAE-BRNS Symposium on Nuclear Physics, Vol. 52, 650 (2007).

Name	:	**Sabyasachi Ghosh**
Enrolment No.	:	PHYS04200704005
Constituent Institute	:	Variable Energy Cyclotron Centre, Kolkatta
Title	:	Probing Spectral Properties of Hadrons in Hot and Dense Hadronic Matter

Abstract

In quark-hadron phase transition, the chiral condensate is one of the order parameter measuring the breaking of chiral symmetry and its study is important to understand the origin or the mass of hadrons. Numerical simulation of QCD thermodynamics on the lattice predict that at high temperature and/or baryon density, this condensate should vanish and chiral symmetry should be restored. It is expected that the resulting changes in the vaccum structure of QCD will affect the correlation functions of vector and axial-vector currents of QCD. They may change in the medium leading to an identical profile at the phase boundary signaling restoration of chiral symmetry. The correlator of vector current of QCD is directly accessible in heavy-ion collisions since it couples to photons and dileptons both of which undergo negligible final-state interaction. In low invariant mass, this is proporational to the spectral function of the low lying vector mesons. The change of the spectral properties of vector mesons in hot and dense medium is consequently reflected in the electromagnetic spectra, specially in the invariant mass spectra of lepton pairs.

We have investigated in-medium spectral properties of ρ and ω mesons by calculating their one-loop self-energy at finite temperature and density. All the branch cuts and the associated discountinuities of the self-energy functions have been discussed in details. The framework of real time thermal field theory that we use, enables us to evaluate the imaginary part of the self-energy from the branch cuts for real and positive values of energy and momentum without having to resort to analytic continuation as in the imaginary time approach. In addition to the unitary cut, present already in the vaccum amplitude, the thermal amplitude generates a new, so-called Landau cut. An extensive set of spin one-half and three-half 4-star resonances in the baryonic loops are taken with the full relativistic baryon propagator in the loop diagrams. The novelty of this full relativistic approach is that the baryons and anti-baryons naturally appear on an equal footing and the additional singularities which are not considered in the Lindhard function approach are automatically included. For the spin 3/2 resonances, an extra term, contributing only in off-mass shell, is added to the Lagrangian because a symmetry is associated with a point transformation under which the free Lagrangian for the Rarita-Schwinger field remains invariant up to a change in the value of its free parameter. Along with the baryon loops, we have included relevant meson loops to get a full modified spectral function of ρ and ω. An almost flattened spectral density of ρ followed by ω Is found at very high temperature and density.

The integrated yield after space-time evolution using relativistic hydrodynamics with quark gluon plasma in the initial state leads to a very good agreement with the experimental data from In-In collisions obtained by the NA60 collaboration. The variation of the inverse slope of the transverse mass (M_T) distribution can be used as an efficient tool to predict the presence of two different phases of the matter during the evolution of the system. The sensitivities of the effective temperature obtained from the slopes of the M_T spectra to the medium effects are studied.

With the help of the same frame work we have studied two other hadrons – nucleon (N) and D meson. Using full relativistic baryon propagator as internal line, our nucleon spectral function differs from the one in non-relativistic approximation, used in some earlier calculations. By taking D meson as a probe of the strongly-interacting matter, we have studied its spectral as well as transport properties with the help of covariant formalism of heavy meson chiral perturbation theory.

Publications

Refereed Journals:

1. Observing many body effects on lepton pair production from low mass enhancement and flow at RHIC and LHC energies. Sabyasachi Ghosh, Sourav Sarkar, Jan-e Alam (VECC, India). Eur. Phys. J. C 71 (2011) 1760. e-print : arXiv:1009.1260v2 [nucl-th].

2. ⬚⬚self energy at finite temperature and density in the real-time formalism Sabyasachi Ghosh, Sourav Sarkar (VECC, India). Nucl. Phys. A 870 (2011) 94 e-print : arXiv:1109.2773v1 [nucl-th].

3. Dragging D mesons by hot hadrons. Sabyasachi Ghosh, Santosh K Das, Sourav Sarkar, Jan-e Alam (VECC, India). Phys. Rev. D 84 (2011) 011503 (R). e-print : arXiv:1104.0163v3 [nucl-th].

4. Baryonic loop in the rho-meson self-energy. Sabyasachi Ghosh, Sourav Sarkar, (VECC, India) , S. Mallik (SINP, India). Phys. Rev. C 83 (2011) 018201.

5. Relativistic spectral function of nucleon in hot nuclear matter. Sabyasachi Ghosh, Sourav Sarkar, (VECC, India) , S. Mallik (SINP, India). Phys.Rev.C 82 (2010) 045202. e-print : arXiv:1004.2162v2 [hep-ph].

6. Analytic structure of _ meson propagator at finite temperature. Sabyasachi Ghosh, Sourav Sarkar, (VECC, India) , S. Mallik (SINP, India). Eur. Phys. J. C 70 (2010) 251. e-print : arXiv:0911.3504v4 [hep-ph].

7. Drag coefficient of B mesons in hot hadronic matter. Santosh K das, Sabyasachi Ghosh, Sourav Sarkar, Jan-e Alam (VECC, India). Phys.Rev.D 85 (2012) 074017. e-print : arXiv:1109.3359v3 [hep-ph].

8. Elliptic flow of thermal dileptons as a probe of QCD matter. Payal Mohanty, Victor Roy, Sabyasachi Ghosh, Santosh K. Das, Bedangadas Mohanty, Sourav Sarkar, Jane Alam, Asis K. Chaudhuri (VECC, India). Phys. Rev. C 85 (2012) 031903 (R). e-print : arXiv:1111.2159v2 [nucl-th].

9. Effect of spectral modification of _ on shear viscosity of a pion gas. Sukanya Mitra, Sabyasachi Ghosh, Sourav Sarkar (VECC, India). Phys. Rev. C 85 (2012) 064917 e-print : arXiv:1204.2388v1 [nucl-th].

Arxiv Submission:

1. Analysis of ! self-energy at finite temperature and density in the real- time formalism Sabyasachi Ghosh, Sourav Sarkar (VECC, India). e-print : arXiv:1207.2251v1 [nucl-th] Conference Proceedings in Journals:

2. The _ meson in hot hadron matter and low mass dilepton spectra. Sabyasachi Ghosh, Sourav Sarkar, Jan-e Alam (VECC, India). Nucl. Phys. A 862 (2011) 294. e-print : arXiv:1101.5946v1 [nucl-th].

3. In-medium vector mesons and low mass lepton pairs from heavy ion collisions. Sourav Sarkar, Sabyasachi Ghosh (VECC, India) Journal of Physics: Conference Series 374 (2012) 012010. e-print : arXiv:1204.0893v1 [nucl-th].

Conference Proceedings:

1. Propagation of rho meson in hot hadronic matter. Sabyasachi Ghosh, Sourav Sarkar, (VECC, India) , S. Mallik (SINP, India). Proceedings of DAE Symp. on Nucl. Phys. (India) 55 (2010) 632.

2. Spectral properties of nucleon in hot nuclear matter. Sabyasachi Ghosh, Sourav Sarkar, (VECC, India) , S. Mallik (SINP, India). Proceedings of DAE Symp. on Nucl. Phys. (India) 55 (2010) 634.

3. In-medium _ mesons, dilepton spectra and flow in heavy ion collisions Sabyasachi Ghosh, Sourav Sarkar, Jan-e Alam (VECC, India). Proceedings of DAE Symp. on Nucl. Phys. (India) 55 (2010) 592.

4. Dragging D by hot hadrons. Sabyasachi Ghosh, Santosh K Das, Sourav Sarkar, Jan-e Alam (VECC, India). Proceedings of DAE Symp. on Nucl. Phys. (India) 56 (2011) 974.

5. Baryonic loops in the _ self energy at finite temperature and density Sabyasachi Ghosh, Sourav Sarkar (VECC, India). Proceedings of DAE Symp. on Nucl. Phys. (India) 56 (2011) 990.

6. Spectral properties of charmed mesons at finite temperature. Sabyasachi Ghosh, Sukanya Mitra, Sourav Sarkar (VECC, India). Proceedings of DAE Symp. on Nucl. Phys. (India) 56 (2011) 918.

7. Transport coefficients of B mesons in hot hadronic matter. Santosh K Das, Sabyasachi Ghosh, Sourav Sarkar, Jan-e Alam (VECC, India). Proceedings of DAE Symp. on Nucl. Phys. (India) 56 (2011) 944.

8. Probing Elliptic Flow of QCD Matter by Lepton Pairs Payal Mohanty, Victor Roy, Sabyasachi Ghosh, Santosh K Das, Bedangadas Mohanty, Sourav Sarkar, Jan-e Alam, Asis K Chaudhuri (VECC, India). Proceedings of DAE Symp. on Nucl. Phys. (India) 56 (2011) 910.

Name : **Yogesh Verma**
Enrolment No. : PHYS03200704004
Constituent Institute : Raja Ramanna Centre for Advanced Technology, Indore:
Title : Biomedical Imaging Using Optical Coherence Tomography

Abstract

In this chapter we provide an overview of the optical imaging methods and highlight the advantages offered by these over the current frontline biomedical imaging modalities like ultrasound, magnetic resonance imaging, etc. We also discuss the basic theory of OCT and review the present state of the art of the OCT technology.

In this chapter we first describe the time domain OCT setup developed by us. The results of our investigation on the use of tapered fiber tip for enhancing the lateral resolution of the OCT setup without significantly compromising the depth of imaging is discussed next. Finally, we describe the development of polarisation sensitive time domain setup to image the birefringent constituents (collagen, tendon, etc.) of the tissue in addition to the structural features of the tissue.

For clinical applications of OCT and for reducing motion-artefact during imaging of living objects, high-speed image acquisition is essential. In this chapter we first describe the development of a high speed OCT setup by incorporation of a rapid scanning Fourier domain optical delay line (FDODL) in TDOCT system (discussed in chapter 2) to achieve image acquisition at 8 frames per second (with 500 A-cans per image). Development of a more sophisticated Fourier domain OCT imaging setup with image acquisition speed of 10 frames per second (with 1000 A-cans per image) and a better signal to noise ratio is discussed next.

In this chapter we describe the results of our studies on the utilization of TDOCT setups for non-invasive, high resolution imaging of the different organs of\ Zebrafish, a vertebrate model system widely used for studies on ocular development and a variety of human diseases. The ocular images obtained using TDOCT setups could be used to measure corneal and retinal thickness and refractive index profile of the lens. A three dimensional iso-surface model of Zebrafish brain was also reconstructed using high resolution (~ 20 μm) two dimensional OCT images and the major structures of the brain could be clearly seen.

In this chapter we describe the use of OCT for quantitative assessment of the birefringence and elastic properties of resected human breast tissue samples. The estimated values of birefringence obtained from the PSOCT imaging showed that the benign breast tissue samples have significantly higher birefringence as compared to the malignant tissue samples. Further, using OCT based elastography measurements, the stiffness coefficients of these tissue samples were also quantified. A significant difference in the stiffness coefficients of the three breast pathologies, normal, benign and malignant, was observed. The use of OCT to monitor the growth dynamics of tumor spheroid noninvasively is also discussed. Here, the study showed that in comparisons with microscopy (which provides only 2D information) the volume estimates provided by OCT were in much better agreement with the total cell count of tumor spheroids measured using hemocytometer.

In this chapter we first describe the use of PSOCT imaging of tissues resected from Staphylococcus aureus infected and uninfected wounds, at different healing times, to assess the morphological changes and collagen remodeling at various stages of wound healing. Next we describe the use of a time domain real time (~ 8 frames/s) OCT set up for monitoring the healing of wounds non-invasively without sacrificing the animal. These measurements showed that compared to the uninfected wounds, the

infected wounds had prominent edematic regions which leads to a significant delay in re-epithelization and collagen remodeling phases of wound healing. The OCT measurements were found to be consistent with the corresponding histological measurements demonstrating the potential of OCT for non-invasive monitoring of the progression of wound healing.

In this chapter we describe the use of a common path phase sensitive FDOCT set up. The phase measurements of interference spectrum fringes, acquired with common path FDOCT setup, were used to achieve optical path length measurements with resolution of ~2 nm. The setup has been used for the measurement of refractive index of biomimetic materials (glucose solution in water having intralipid as the scattering medium) and single biological cells (keratinocyte).

Publications

Journals Articles (Included in the thesis)

1. Use of common path phase sensitive spectral domain optical coherence tomography for measurement of refractive index. Y. Verma, P. Nandi, K. D. Rao, M. Sharma, and P. K. Gupta *App. Opt.50, E7-E12 (2011).*

2. Determination of elastic properties of resected human breast tissue samples using optical coherence tomographic elastography. A. Srivastava, Y. Verma, K. D. Rao and P. K. Gupta *Strain 47, 75–87 (2011).*

3. Imaging of human breast tissue using polarisation sensitive optical coherence tomography Y. Verma, M. Gautam, K. D. Rao, M. K. Swami and P. K. Gupta *Laser Physics 21, 2143-48, (2011).*

4. Non-invasive assessment of healing of bacteria infected and uninfected wounds using optical coherence tomography. K. Sahu, Y. Verma, M. Sharma, K. D. Rao, P. K. Gupta. *Skin research and technology 16, 428 (2010)*

5. Real-time *in-vivo* imaging of adult Zebrafish brain using optical coherence tomography. K. D. Rao, A. Alex, Y. Verma, S. Thampi, P. K. Gupta *J Biophotonics. 2(5):288-91, (2009).*

6. Optical coherence tomography using a tapered single mode fiber tip. Y. Verma, K. Divakar Rao, S. K. Mohanty, and P.K. Gupta. *Laser Physics Letters, 4, 686-689 (2007)*

7. Measurement of gradient refractive index profile of crystalline lens of fisheye *in-vivo* using optical coherence tomography. Y. Verma, K. D. Rao, M. K. Suresh, H.S. Patel and P.K. Gupta *Applied Physics B. 87, 607-610 (2007)*

8. Imaging growth dynamics of tumor spheroids using optical coherence tomography. M. Sharma, Y. Verma, K. D. Rao, R. Nair and P. K. Gupta. *Biotechnology Letters, 29, 273-278 (2007).*

9. Non-invasive ophthalmic imaging of adult Zebrafish eye using optical coherence tomography. K. D. Rao, Y. Verma, H. S. Patel and P. K. Gupta, *Current Science, 90, 1506, (2006)*

Not included in the thesis)

10. Single mode fiber based polarization sensitive optical coherence tomography using swept laser source. P. Sharma, Y. Verma, K. D. Rao, and P. K. Gupta, *Journal of Optics 13, 115301-06 (2011).*

11. Binary tissue classification studies on resected human breast tissues using optical coherence tomography images. M. Bhattachrjee, P. C. Ashok, K. D. Rao, S. K. Majumder, Y.Verma, and P.K.Gupta *Journal of Innovative Optical Health Sciences, 4, 59-66 (2011).*

12. Effect of He-Ne laser irradiation on hair follicle growth cycle of swiss albino mice. S.Shukla, K Sahu, Y. Verma, K. D. Rao, A. Dube, and PK Gupta. *Skin Pharmacol Physiol, 23, 79–85 (2010).*

In Edited Volumes:

1. *In-vivo* imaging of adult Zebrafish using optical coherence tomography. Y. Verma, K. D. Rao, A. Alex, and P. K. Gupta Proc. SPIE OCT Microscopy, 71390H (2008); DOI:10.1117/12.814914.

2. Effect of He-Ne laser irradiation on hair follicle growth in testosterone treated mice investigated with optical coherence tomography and histology. Shukla, Y. Verma, K. Sahu, K. D. Rao, A. Dube, and P. K. Gupta *KIRAN (A Bulletin of Indian Laser Association), Vol. 19, no.1, p. 31-34, 2008.* The paper was adjudged by ILA as one of the five best posters presented at NLS-07.

3. apered single mode fiber tip for high lateral resolution imaging in Optical Coherence Tomography. Y. Verma, K. D. Rao, S. K. Mohanty and P. K. Gupta. *The International Biomedical Optics Symposium (BiOS) San Diego USA, SPIE p. 64360Y, 2007.*

4. Optical Coherence Tomography. K. D. Rao, Y. Verma and P. K. Gupta *KIRAN (A Bulletin of Indian Laser Association), Vol. 17, no.3, p. 69-74 , 2006.* Conference Presentations / Publications:

5. Use of common path phase sensitive spectral domain optical coherence tomography setup for refractive index measurements. Y. Verma, P, Nandi, K. D. Rao, M. Sharma, and P. K. Gupta. *International conference on opto-electronics, fiber optics and photonics, held at Guwahati, December 2010.*

6. Swept source based fiber optic polarization sensitive optical coherence tomography setup for tissue birefringence. P. Sharma, Y. Verma, K. D. Rao, and P. K. Gupta *International conference on opto-electronics, fiber optics and photonics, held at Guwahati, December 2010.*

7. Combined Raman spectroscopy-optical coherence tomography for analysis of tissue pathology. S. K. Majumder, Y. Verma, K. Divakar Rao, M. K. Swami and P. K. Gupta *International conference on opto-electronics, fiber optics and photonics, held at Delhi, 2009.*

8. Polarization Sensitive Optical Coherence Tomography for Imaging of Human Breast Tissue. Y. Verma, M. Gautam, K. D. Rao, M. K. Swami and P. K. Gupta *Fifth International Symposium on Modern Problems of Laser Physics (MPLP) August 24-30, 2008, p 199-200, Novosibirsk, Russia.*

9. A new approach for mueller matrix measurement using fiber based optical coherence tomography. M. K. Swami, Y. Verma, S. Manhas, K. D. Rao, N. Ghosh and P. K. Gupta. *International Conference on Optics within Lifesciences OWLS-10, Biophotonics Asia, July 2-4, 2008, Singapore.*

10. Analysis of optical coherence tomography images for binary classification of resected human breast tissues. K. D. Rao, P. C. Ashok, M. Bhattacharjee, Y. Verma, S. K. Majumder and P. K. Gupta *International Conference on Optics within Lifesciences OWLS-10, Biophotonics Asia, July 2-4, 2008, Singapore.*

11. Polarization Sensitive Optical Coherence Tomography using a single detector and dual reference beams. Y. Verma, M. K. Swami, K. D. Rao and P.K. Gupta. *Saratov Fall Meeting (SFM), September 25-28,2007, Saratov, Russia.*

12. Effect of He-Ne laser irradiation on hair follicle growth in testosterone treated mice investigated with optical coherence tomography and histology. S. Shukla, Y. Verma, K. Sahu, K. D. Rao, A. Dube, and P. K. Gupta. *Proc. DAE-BRNS National Laser Symposium, December 17-20, 2007, Vadodara.*

13. Tapered single mode fiber tip for high lateral resolution imaging in Optical Coherence Tomography. Y. Verma, K. D. Rao, S. K. Mohanty and P. K. Gupta. *BIOS San Diego USA 2007.*

14. Non-invasive measurement of graded refractive index profile of Zebra fish lens *invivo* using Optical Coherence Tomography. Y. Verma, K. D. Rao, M. K. Suresh, H. S. Patel and P. K. Gupta. *Eighth international conference on opto-electronics, fiber optics and photonics, held at Hyderabad, December 2006.*

15. Imaging growth dynamics of tumour spheroids using optical coherence tomography. M. Sharma, Y. Verma, K. D. Rao, R. Nair and P. K. Gupta. *Eighth international conference on opto-electronics, fiber optics and photonics, held at Hyderabad, December 2006.*

Name   :   **Viveka Nand Singh**
Enrolment No.   :   PHYS08200604016
Constituent Institute   :   Harish-Chandra Research Institute, Allahabad
Title   :   The Impact of Antisite Disorder on Magnetism and Transport in
                                   the Double Perovskites

Abstract

Perovskites are materials of the form ABO_3, while 'double perovskites' (DPs) are of the form $ABO_3.AB'O_3$ = $A_2BB'O_6$. The B and B' are the electronically active ions, typically *3d, 4d or 5d* elements, while *A* is either a rare earth or alkaline earth and controls the valence. It shows a variety of electronic and magnetic phases and some very interesting properties like high ferromagnetic T_c, half-metallic behavior, large low field magnetoresistance (MR) etc. The B ions are usually magnetic, *Fe, Co, Ni, Cr, Mn etc.* while *B'* is typically non-magnetic, e.g., *Mo, W etc*. In the structurally ordered double perovskite the B and B' should alternate along each cubic axis. However, unless the B and B' are very dissimilar ions, there is a significant possibility of mislocation. The B ion can occupy a *B'* site and vice versa. The promise of rich functionality in the DP's remains unfulfilled due to this *B, B'* mislocation. Here we have studied the impact of correlated antisite disorder (ASD), on magnetism and transport in the DPs.

We describe the use of a simple "lattice-gas" model for the structural variables which, on poor annealing, generates a domain structure mimicking the antisite pattern. The electronic-magnetic model is defined on this structural motif and solved via a real space Monte Carlo technique involving the "travelling cluster" algorithm.

In the ferromagnetic (FM) phase, for ASD with a high degree of short-range correlations, the antiphase boundaries act also as magnetic domain walls. Increasing ASD reduces the low-field magnetization, destroys the half-metallicity, and makes the ground state insulating. While these are disadvantages, we also note that the ferromagnetic T_c is only weakly affected by moderate ASD and the low-field MR is dramatically enhanced by disorder. Our real space approach allows an interpretation of these results in terms of the domain pattern, the effective exchange, and the short-range magnetic correlations. They are also consistent with explicit spatial imagery from recent experiments. The "intra-grain" effects highlighted here would be directly relevant to single crystals, and define the starting point for a transport theory of the polycrystalline DPs.

On electron doping the FM DPs shows the metallic antiferromagnetic (AFM) phase. For spatially correlated ASD the AFM order is affected much less strongly than in the FM case. This intriguing result arises from the finite **Q** nature of AFM order which leads to a weaker 'cancellation' of the order between domains. So, despite the possibility of large ASD in the electron doped DPs, there is certainly hope of observing AFM phases. The AFM states are metallic, and the electronic wavefunctions in these phases continue to be spatially extended even at large disorder. ASD increases the residual resistivity, but, unlike the ferromagnet, we do not observe insulating phase.

While the zero field resistivity is unremarkable in the AFM DP metals, they have huge positive MR. In contrast to elaborate structure factor measurements etc., this is a direct indicator of the metallic AFM

system. Beyond a modest field needed for suppression of long range AFM order, the system shows more than ten-fold increase in resistivity near T_c in a structurally ordered system. The ratio continues to be almost two-fold even in systems with 25% ASD. An applied field suppresses long range AFM order leading to a state with short range AFM correlations in the field induced FM background. These AFM fluctuations generate strong electronic scattering and a resistivity that can be much larger than the ordered AFM metal. Although our explicit demonstration is in the context of a two dimensional spin-fermion model of the DPs, the mechanism we uncover is far more general and complementary to the colossal negative MR process. It should operate in other local moment metals that show a field driven suppression of non FM order.

We have studied the magnon spectrum in domain FM state of antisite disordered DPs. The results on magnon energy and broadening reveal that even at very large disorder, the existence of domain like structure ensures that the response has a strong similarity to the clean case. We tried out a scheme for inferring the domain size from the spin wave damping so that experimenters can make an estimate of domains without having spatial data, and we find it to be reasonably successful. We also highlight how the common assumption about random antisites, which is widely used in modeling these materials, would lead to a gross overestimate of magnon damping. In summary, dynamical neutron scattering can be a direct probe of the unusual FM state in these materials and confirm the presence of correlated antisites.

To summarise, this thesis considers some problems in the antisite disordered DP magnets. We clarify the impact of correlated ASD on both FM and AFM phases, discover that the antiferromagnet is robust to large disorder, and find that the AFM metal has a surprisingly large positive MR. Finally, we have provided results on the magnon spectrum in the non trivial domain FM phase and provide an interpretation of the spectrum in terms of magnon confinement.

Publications

1. Antisite Domains in Double Perovskite Ferromagnets: Impact on Magnetotransport and Half-metallicity Viveka Nand Singh and Pinaki Majumdar Europhys. Lett. 94, 47004 (2011), arXiv: 1009.1702 (2010).

2. Antiferromagnetic Order and Phase Coexistence in a Model of Antisite Disordered Double Perovskites Viveka Nand Singh and Pinaki Majumdar Eur. Phys. J. B 83, 147-155 (2011), arXiv: 1009.1709 (2010).

3. Huge Positive Magnetoresistance in Antiferromagnetic Double Perovskite Metals Viveka Nand Singh and Pinaki Majumdar arXiv: 1107.0782 (2011).

4. The Magnon Spectrum in the Domain Ferromagnetic State of Antisite Disordered Double Perovskites Subrat Kumar Das, Viveka Nand Singh, and Pinaki Majumdar arXiv: 1204.1194 (2012).

5. Thermally Fluctuating Inhomogeneous Superuid State of Strongly Interacting Fermions in an Optical Lattice Viveka Nand Singh, Sanjoy Datta, and Pinaki Majumdar arXiv: 1104.4912 (2011). The material in papers 1-4 above is discussed in the thesis.

Name	:	**Amit Kumar Bhattacharjee**
Enrolment No.	:	PHYS10200604009
Constituent Institute	:	Institute of Mathematical Science, Chennai
Title	:	Inhomogeneous Phenomena in Nematic Liquid Crystals

Abstract

This thesis addresses problems involving inhomogeneous order parameter configurations at a phase transition between isotropic and nematic phases in liquid crystals. We propose new fluctuating equations and accurate numerical algorithms for this class of problems. We apply our methods to study the nematic-isotropic interface, the spinodal kinetics, and the growth of droplets in nucleation. The formalism of Landau-Ginzburg theory and the time-dependent relaxational equations provide a coherent approach to understand inhomogeneous phenomena in nematic liquid crystals. In this thesis, we promote the time-dependent Ginzburg-Landau (TDGL) equations to Langevin equations by adding noise terms which preserve the symmetry and tracelessness of the order parameter. We then develop efficient numerical methods, based on the method of lines (MOL) for solving both deterministic and stochastic TDGL equations. We develop a spectral collocation scheme for obtaining the steady-state solutions of the TDGL equations. The numerical methods are benchmarked by comparing our results with analytical and, when available, previous numerical results.

In the structure of isotropic - uniaxial nematic interface, we show that provided elastic anisotropy is absent, the classical de Gennes ansatz is valid. When anisotropy is present, the interface becomes biaxial for any anchoring condition other than homeotropic. For oblique anchoring condition, the spatial variations of the scalar order parameters are largely confined to the neighbourhood of the interface, while director orientations interpolate smoothly between the planar or homeotropic anchoring selected at the interface to the imposed orientation at the boundary. We devise a simple way of identifying point defects from the suppression of the scalar order. We find that half-integer charge defects are stable at late stages of the dynamics while integer charge defects appear only at the early stage. We also develop visualization methods for studying the dynamics of topological defects & we find clear signature of the intercommutation of defect lines. We also show that dynamical scaling holds, with a diffusive growth. We find agreement with Porod's law obtained at intermediate and late stages of the dynamics, governed principally by defect-antidefect annihilation processes. We also recover a diffusive growth at the very late stage of dynamics. In addition, we also study the effects of thermal fluctuations on the defect density.

In nucleation kinetics, we show that in the presence of elastic anisotropy (denoted as k), an initially spherical uniaxial nematic nucleus immersed in an isotropic background changes shape to an ellipsoid, with the long axis oriented depending on the sign of k. In two dimensions and in the presence of thermal fluctuations, two regimes are observed, depending on the sign of k. For k>0, integer charged defects develop inside the nematic bubble with ellipsoidal shapes. The defects remain even at late stages of the dynamics, by which time bubbles have coalesced completely and the nematic phase fluctuates in equilibrium. For k<0, a uniform director field emerges but the bubbles are observed to be ellipsoidal. Without the anisotropic elastic term, circular nematic bubbles nucleate with uniform director configuration. Classical nucleation theory is thus inapplicable in the case of both k>0/k<0 since the order parameter configurations can be non-uniform and the droplet shape is far from being spherical.

Publications:

1. Numerical method of lines for the relaxational dynamics of nematic liquid crystals. Bhattacharjee, Menon and Adhikari, *Phys. Rev. E*, **78**, 026707 (2008).

2. Biaxiality at the isotropic - nematic interface with planar anchoring. Kamil, Bhattacharjee, Adhikari, Menon, *Phys. Rev. E*, **80**, 041705 (2009).

3. The isotropic-nematic interface with an oblique anchoring condition. Kamil, Bhattacharjee, Adhikari, Menon, *J. Chem. Phys.*, **131**, 174701 (2009).

4. Fluctuating dynamics of nematic liquid crystals using the stochastic method of lines. Bhattacharjee, Menon, Adhikari, *J. Chem. Phys.*, **133**, 044112 (2010).

Name   :   **Ritesh Ruhela**
Enrolment No.   :   CHEM01200804013
Constituent Institute   :   Bhabha Atomic Research Centre, Mumbai
Title   :   Inhomogeneous Phenomena in Nematic Liquid Crystals

Abstract

Separation and recovery of palladium from high level liquid waste (HLLW) is necessary from the viewpoint of various problems encountered during vitrification as well as the conceptualization of the process where HLLW can be treated as a secondary source of this valuable metal.

Novel ligands, namely, N,N,N',N'-tetra-(2-ethylhexyl) thiodiglycolamide (T(2EH)TDGA) and N,N,N,',N'-tetra-(2-ethylhexyl) dithiodiglycolamide (DTDGA) have been synthesized, characterized and evaluated for the extraction behavior of Pd and metal ions present in HLLW. Both the ligands have shown very shown very high extractability and selectivity for Pd, with the later giving the highest D_{pd} reported so far in the literature. The structural investigation of Pd(II)- T(2EH)TDGA and Pd(II)-DTDGA complexes has been carried out by EXAFS and DFT studies.

Novel ligand grafted polymeric resins, namely, AP-XAD16 have been synthesized, characterized and evaluated for separation of Pd from HLLW. AP-XAD16 resin have high extractability and selectivity for Pd over other metal ions present in HLLW and can be used for separation and recovery of Pd. ACAM-XAD16 resin have shown co-extraction of lanthanides along with Pd and therefore can apply be used after actinide partitioning.

Publications

1. *N,N,N',N'*-tetra-(2-Ethylhexyl) Thiodiglycolamide T(2EH)TDGA: A Novel Ligand for Separation and Recovery of Palladium from High Level Liquid Waste (HLLW) Solutions. R. Ruhela, J.N. Sharma, B.S. Tomar, S. Panja, S.C. Tripathi, R.C. Hubli, A.K. Suri. Radiochimica Acta, 2010, 98, 209-214.

2. *N,N,N',N'*-tetra-(2-Ethylhexyl)Thiodiglycolamide (T(2EH)TDGA): A Promising Ligand for Separation and Recovery of Palladium from High Level Liquid Waste (HLLW) Solutions. R. Ruhela, J.N. Sharma, B.S. Tomar, V.C. Adya, T.K. Sheshgiri, R.C. Hubli, A.K. Suri. Separation Science & Technology, 2011, 46, 1-7.

3. Extractive spectrophotometric determination of palladium with *N,N,N',N'*-tetra-(2- ethylhexyl)-thiodiglycolamide T(2EH)TDGA. R. Ruhela, J.N. Sharma, B.S. Tomar, R.C. Hubli, A.K. Suri. Talanta, 2011, 85 (2), 117-1220.

4. Dithiodiglycolamide: Novel ligand with highest selectivity and extractability for palladium. R. Ruhela, J.N. Sharma , B.S. Tomar , M.S. Murali , R.C. Hubli, A.K. Suri. Tetrahedron Letters, 2011, 52, 30, 3929-3932.

5. Studies on hydrolysis and radiolysis of *N,N,N',N'*-tetra-(2-ethylhexyl)thiodiglycolamide T(2EH)TDGA. R. Ruhela, J.N. Sharma, B.S. Tomar, K.K. Singh, M. Kumar, R.C. Hubli, A.K. Suri. Radiochimica Acta, 2012, 100, 37-44.

6. Studies on Separation and Recovery of palladium from Simulated High Level Liquid Waste (SHLW) Solution with novel extractant *N,N,N',N'*-tetra-(2-ethylhexyl)- dithiodiglycolamide DTDGA. R. Ruhela, B.S. Tomar, J.N. Sharma, T.K. Sheshgiri, V.C. Adya, R.C. Hubli, A.K. Suri. Separation Science & Technology, 2012, (DOI: 10.1080/01496395.2012. 724 140). 159

7. Stability Studies of *N,N,N',N'*-tetra-(2-ethylhexyl) dithiodiglycolamide (DTDGA). R. Ruhela, B.S. Tomar, K.K. Singh, J.N. Sharma, M. Kumar, P.N. Bajaj, V.C. Adya, T.K. Seshagiri, R.C. Hubli, A.K. Suri. Radiochimica Acta, 2012 (DOI: 10.1524/ract.2013.2008).

8. Amberlite XAD-16 functionalized with 2-acetyl pyridine group for the solid phase extraction and recovery of palladium from High Level Waste (HLW). R. Ruhela, K.K. Singh, B.S. Tomar, J.N. Sharma, M. Kumar, R.C. Hubli and A.K. Suri. Separation and Purification Technology, 2012, 99, 36–43.

9. Separation and Recovery of Palladium from Spent Nuclear Fuel – a Review. R. Ruhela, B.S. Tomar, J.N. Sharma, R.C. Hubli, A.K. Suri. Communicated. 10. Amberlite XAD-16 functionalized with 2-Acetyl Amide group for the solid phase extraction and recovery of palladium from High Level Waste (HLW). R. Ruhela, K.K. Singh, B.S. Tomar, T.K. Seshagiri, M. Kumar, R.C. Hubli, A.K. Suri. Communicated.

10. Investigation of the Extraction Complexes of Palladium (II) with Novel Ligands Thiodiglycolamide and Dithiodiglycolamide by EXAFS and Computational Methods. R. Ruhela, B.S. Tomar, A.K. Singh, R.C. Hubli, A.K. Suri. Communicated.

Name	:	**Nishita Desai**
Enrolment No.	:	PHYS08200604022
Constituent Institute	:	Harish-Chandra Research Institute, Allahabad
Title	:	Signals of Supersymmetry and Higgs at the Large Hadron Collider

Abstract

My Ph.D thesis focuses on phenomenological studies and addresses two questions. First that of looking for Supersymmetry (SUSY) by detecting squarks of the third generation (in theories both with and without R-parity). The problem of Higgs mass stabilisaion is solved in theories with SUSY by the cancellation of the corrections to the Higgs mass from the top and stop (top-squark) loops. To avoid fine-tuning. We would require stop mass to be within a TeV, and hence, we expert stops to be produced at the LHC. Search for top-squarks is therefore a robust way to searching for Supersymmetry.

Secondly, I address the question of determining Higgs coupling to guage bosons. Assuming that a Higgs-like resonance is observed at the LHC, the next step will be to confirm whether it indeed corresponds to the Standard Model (SM) Higgs. For this, one needs to measure its coupling to gauge bosons since it is here that the structure of the underlying theory will be reflected. I propose a solution the question of measuring any anomalous contribution to the HWW vertex and to pinpoint its CP property.

Publications

1. Signals of supersymmetry with inaccessible first two families at the Large Hadron Collider. Nishita Desai, Biswarup Mukhopadhyaya Phys. Rev. D 80, 055019 (2009) [arXiv:0901.4883]

2. R-parity violating resonant stop production at the Large Hadron Collider Nishita Desai, Biswarup Mukhopadhyaya JHEP 1010 (2010) 060. [arXiv:0102.2339]

3. CP-violating HWW couplings at the Large Hadron Collider Nishita Desai, Dilip Kumar Ghosh, Biswarup Mukhopadhyaya Phys. Rev. D 83, 113004 (2011) [arXiv:1104.3327]

4. Constraints on supersymmetry with light third family from LHC data Nishita Desai, Biswarup Mukhopadhyaya *Preprint* [arXiv:1111.2830] *Submitted to JHEP*

Other Publications

1. Supersymmetry and Generic BSM Models in PYTHIA 8 Nishita Desai and Peter Skands *Preprint* [arXiv:1109.5852]

Name	:	**Kamalakanta Satpathy**
Enrolment No.	:	PHYS02200704003
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	Studies on Prediction of Gas Entrainment Inception in Hot Pool of Liquid Metal Fast Reactors

Abstract

In Fast Breeder Reactor (FBR), the sodium pool is blanketed by inert argon cover gas, (i) to avoid Sodium-air contact through penetrations in the roof-slab, (ii) to act as a cushion for accommodating sodium volume changes due to plant transients and (iii) to reduce the heat load to roof-slab. Due to compact layout of reactor system, sodium velocity in the pool is generally high, which leads to local fluid swell in pool and vortex formation around reactor components partially submerged in sodium and partially exposed to argon gas. These are sources of argon entrainment into liquid sodium, which is an important safety problem in nuclear industry. The focus of the research work is to identify the free surface criteria for onset of gas entrainment and its mitigation. As a part of this research, fundamental Computational Fluid Dynamics (CFD) studies on idealized hot pool models have been carried out employing the Volume of Fluids (VOF) method, to understand free surface characteristics, Viz., free surface velocity magnitude and argon-sodium interface profile and their role in argon gas entrainment. Following this, a suitable design provision for the hot pool of Indian FBR has been identified and the same has been implemented in the reactor. Also, basic studies on 3-D vortex shedding behind cylindrical components partially submerged in sodium pools have been carried out for laminar and turbulent regimes. The effect of bed friction on vortex shedding characteristics has been brought out. Interactions between free surface waves and underlying viscous wake are investigated for turbulent flow past a free surface piercing circular cylinder at various Reynolds numbers using SST k-w model.. The mathematical models adopted in the research work employing the FLUENT code have been validated against published benchmark dada.

Publications

1. K. Satpathy, K. Velusamy, B.S.V. Patnaik, P. Chellapandi, Numerical investigation of vortex shedding past a finite circular cylinder mounted on a flat plate, *Numerical Heat Transfer-A*, 59(11), 882 – 909, 2011.

2. K. Satpathy, K. Velusamy, P. Chellapandi, Computational fluid dynamic studies on gas entrainment in fast breeder reactors, *Energy Procedia*, 7, 333 – 339, 2011.

3. K. Velusamy, P. Chellapandi K. Satpathy, N. Verma, G.R. Raviprasan, M. Rajendrakumar, S.C. Chetal, A fundamental approach to specify thermal and pressure loadings on containment buildings of sodium cooled fast reactors during a core disruptive accident, *Annals of Nuclear Energy*, 38, 2475 – 2487, 2011.

4. K. Satpathy, K. Velusamy, B.S.V. Patnaik, P. Chellapandi, Numerical simulation of liquid fall induced gas entrainment and its mitigation, *International Journal of Heat and Mass Transfer* (Revised version submitted to the Editor).

5. K. Satpathy, K. Velusamy, B.S.V. Patnaik, P. Chellapandi, Gas entrainment at free surface of a pool during cross flow over partially submerged component, (communicated).

Conference Proceedings

1. K. Satpathy, K. Velusamy, P. Chellapandi, Condensation behaviour of fuel vapour in sub-cooled liquid sodium during a severe accident in a fast breeder reactor, *International Conference on Modeling and Simulation*, Coimbatore, India, 27th – 29th August 2007.
   K. Satpathy, K. Velusamy, P. Chellapandi, Computational fluid dynamic studies on gas entrainment in fast breeder reactors", , *2nd International Conference on Asian Nuclear Prospects (ANUP-2010)*, Mamallapuram, Chennai, India, 11th -13th October 2010.

2. K. Satpathy, K. Velusamy, B.S.V. Patnaik, P. Chellapandi, CFD simulation of gas entrainment in a liquid pool by VOF method, *Proceedings of the 4th International* 155 *Conference on Fluid Mechanics and Fluid Power*, IIT-Madras, India, 16th - 18th December 2010.

3. K. Satpathy, K. Velusamy, B.S.V. Patnaik, P. Chellapandi, Investigation of argon gas entrainment in liquid sodium at free surface during cross flow over cylindrical components, *IUTAM-2011*, IIT-Kanpur, India, 12th -16th December 2011.

IGCAR Design Reports

1. Condensation time and migration height of core bubble in primary sodium during a CDA, PFBR/31050/DN/1000/R-A/2010.

2. Benchmarking of OpenFOAM based CFD tool: study- numerical simulation of flow around bluff bodies, PFBR/30000/DN/1106/R-A/2010.

3. Effect of welding of anti-gas entrainment baffle on inner vessel, PFBR/31240/DN/1016/RA/ 2010/R-A/2011.

4. Optimization of anti-gas entrainment baffle attached to inner vessel, PFBR/32100/DN/1012/R-A/2011.

5. Effect of manufacturing deviation in inner vessel on hot-pool thermal hydraulics, PFBR/32100/DN/1013/R-A/2011.

6. Benchmarking Of OpenFOAM Based CFD Tool: Study–2, PFBR/30000/DN/1110/RA/ 2012.

Name	:	**Sumit Kumar**
Enrolment No.	:	CHEM01200604015
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Equilibrium and Kinetic Studies of Sorption of Actinides and Fission Products at Solid/Liquid Interface

Abstract

As part of the dissertation work, batch sorption study, molecular level spectroscopic techniques, linear additive and surface complexation modelling were employed to investigate the sorption behaviour of actinides and long lived fission products on oxide surfaces and Smectite rich natural clay. Aspects delineated in these studies are (1) effect of humic acid (HA) on sorption of fission products by mineral oxides, (2) role of surface reactivity in defining the speciation of tri- and tetra valent actinides at oxide-water interface, and (3) modelling of sorption of trivalent actinides on smectite rich natural clay. The major findings and conclusions from this work are as follows.

Enhancement in metal ion sorption at oxide surfaces in presence of HA is related to the intrinsic characteristics of HA. Ionic strength effect in Cs(I) sorption on silica indicates that the sorption enhancement in presence of HA is due to electrostatic interaction of Cs(I) with counter charge produced by silica-surface-sorbed HA. Enhancement in case of Tc(IV) sorption on alumina was attributed to complexation of Tc(IV) with surface sorbed HA. Surface complexation modelling showed the formation of a ligand bridged complex of Tc(IV) on HA sorbed alumina surface.

At solid/liquid interface, sorption and speciation of metal ions are majorly decided by the solid surface. Its solubility in pH range and its structural characteristics govern the binding of metal ions. Am/Eu(III) speciation on alumina under varying pH and metal ion concentration showed the formation of mononuclear monodentate surface species at lower metal ion concentration (10^{-6}-10^{-7} M) while mononuclear bidentate species compete with monodentate species at higher metal ion concentration. XAFS investigation of Eu(III) speciation on silica and alumina surfaces under pH and metal ion concentration conditions over and under saturated with respect to $Eu(OH)_3$ precipitation indicated the absence of hydroxide precipitation. Both the surfaces have similar surface speciation of Eu; however, silica favours corner sharing binding while alumina has preference for edge shared binding. Pu(IV) sorption on silica and alumina shows polymerized surface species formed over pH range. In silica supernatant V is the oxidation state of Pu while VI followed by V is Pu oxidation state in alumina supernatant.

Proper consideration of minor components present in the natural substrates and the effect of ground water chemistry under surface complexation modelling could simulate the sorption process in natural systems.

Publications

1. Kumar, S., Tomar, B. S., Manchanda, V. K., Ramanathan, S. (2006) Effect of humic acid on adsorption behaviour of 137Cs on silica colloids, *Radiochim. Acta* 94, 369 – 373.

2. Kumar, S., Rawat, N., Tomar, B. S., Manchanda, V. K., Ramanathan, S. (2007) Effect of humic acid on the sorption of technetium on hematite colloids using 95mTc and 96Tc as tracers, *J. Radioanal. Nucl. Chem.* 274, 229 - 231.

3. Kumar, S., Rawat, N., Kar, A. S., Tomar, B. S., Manchanda, V. K. (2011) Effect of humic acid on sorption of technetium by alumina, *J. Hazard. Mat.* 192, 1040 –1045.

4. Kumar, S., Godbole, S. V., Tomar, B. S., Speciation of Am(III)/Eu(III) sorbed on γ- Alumina: Effect of metal concentration, *Radiochim. Acta*. *DOI No.* 10.1524/ract.2013.1997.

5. Kumar, S., Kar, A. S., Tomar, B. S., Bhattacharya, D. (2012) XAFS Spectroscopy study of Eu(III) sorption products on Amorphous Silica and γ-Alumina: Effect of pH and substrate, *Polyhedron* 33, 33 - 40.

6. Kumar, S., Kasar, S. U., Tomar, B. S. (2012) Interfacial sorption/desorption studies of Pu(IV) on Silica and alumina surfaces, *Radiochim. Acta*. 100, *885 – 892.*

7. Kumar, S., Pente, A. S., Kaushik, C. P., Bajpai, R. K., Tomar, B. S., Americium sorption on smectite rich natural Clay from granitic water, *Appl. Geochem. (under review).*

Name	:	**Rohit Singh Chauhan**
Enrolment No.	:	CHEM01200704003
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Organometallic Chemistry of Platinum Group Chalcogenolates: Synthesis, Structure and Spectroscopy

Abstract

Oxidative addition reactions of diorganodichalcogenides (REER) to platinum(0) and palladium(0) complexes have attracted condsiderable attention due to their application in region and stereo-selective E-E addition to C≡C bonds in organic synthesis and also provides a convenient route to metal chalcogenolate complexes which have relevance in materials science. These complexes are not only used as precursors but also several of them are envisaged as active species in catalytic reactions. On the other hand platinum(0) complexes, due to their superior stability provide an opportunity to understand the mechanistic details and learn about the nature of the complexes involved in such reactions.

In the view of the above, the chemistry of palladium and platinum complexes with hemilabile 2-pyridylchalcogenolate (2-E-C5H4N); (E = S, Se or Te) have been examined in thesis. The reactions of palladium(0) and platinum(0) complexes containing non-chelaing and chelating diphosphines with varying degree of P-M-P angles with dipyridyl dichalcogenides have been investigated. Depending on the nature of chalcogen and phosphine ligand, different products could be isolated. All the complexes have been characterized by elemental analysis, UV-vis and NMR (^{1}H, ^{31}C{^{1}H}, ^{77}Se{^{1}H} ^{125}Te{^{1}H} and ^{195}Pt{^{1}H}) spectroscopy. Molecular structures of [Pt{2-Te-C5H3(Me)N}$_2$Te(PPh$_3$)], [Pt{PPH$_2$C(Te-C$_5$H$_4$N)$_2$PPh$_2$}$_2$], [Pt$_2${TeC$_5$H$_3$(3-Me)N}$_2$(dppe)$_2$] [BPh$_4$]$_2$, [Pd3(μ-Te)2(dppp)3]Cl2 and [PdCl{2-Te(Cl)2C5H3(3-Me)N}(PPh3)] have been elucidated by single X-ray crystallography. The thesis work has resulted in 7 research papers in peer reviewed international journals and 5 symposium/conference papers.

Publications

1. Tellurium(0) as a ligand: Synthesis and characterization of 2-pyridyltellurolates of platinum (II) and structures of [Pt{2-Te-3-(R)C5H3N}2Te(PR'3)] (R = H or Me). R. S. Chauhan, G. Kedarnath, A. Wadawale, A. M. Castro, R. A. Perez, V. K. Jain, W. Kaim *Inorg. Chem.*, 49 (2010) 4179-4185.

2. Reactions of 2-telluropyridine ligands with (diphosphine)Pto and (diphosphine)PtCl2 complexes and isolation of different structural motifs of platinum(II)complexes. R. S. Chauhan, G. Kedarnath, A. Wadawale, A. L. Rheingold, A. M.Castro, R. A. Perez, V. K. Jain *Organometallic*s, 31 (2012) 1743-1750.

3. Reactivity of dipyrimidyldiselenides with [M(PPh3)4] and 2-pyrimidylchalcogenolates with [MCl2(diphosphine)] (M = Pd or Pt) R. S. Chauhan, R. K. Sharma, G. Kedarnath, D. B. Cordes, A. M. Z. Slawin, V. K. Jain *J. Organomet. Chem.*, 717 (2012) 180-186.

4. Reactivity of 2-chalcogenopyridines with palladium-phosphine complexes: Isolation of different complexes depending on the nature of chalcogen atom R. S. Chauhan, G. Kedarnath, A. Wadawale, A. M. Z. Slawin, V. K. Jain *Dalton Trans.*, 42 (2013) 259-269.

5. Oxidative addition reactions of nicotinamide based organoselenium compounds on [M(PPh3)4] (M = Pd or Pt) : An insight study for the formation of several isolable products R. S. Chauhan, C. P. Prabhu, P. P. Phandis, G. Kedarnath, J. A. Golen, A. L. Rheingold, V. K. Jain *J. Organomet. Chem.*, 723 (2013) 163-170.

6. Bis phosphine palladium(II) mesityl chalcogenolate complexes: Synthesis and structure of [Pd(SeMes)2(dppe)] R. S. Chauhan, G. Kedarnath, A. Wadawale, J. A. Golen, A. L. Rheingold, V. K. Jain *Ind. J. Chem.,*52 A (2013) 42-44.

7. Cis configured bis phosphine platinum(II) chalcogenolate complexes: Structures and a comparative NMR study R. S. Chauhan, G. Kedarnath, A. Wadawale, J. A. Golen, A. L. Rheingold, V. K. Jain *J. Organomet. Chem.* (submitted)

Conferences/Symposia

1. Structural and spectroscopic characterization of platinum complex with C-substituted (pyridyltelluro)-bis(diphenylphosphino)methane, R. S. Chauhan, G. Kedarnath, A. Wadawale, V. K. Jain "3rd International Conference on Materials Chemistry", 7-10 December 2010, BARC, Mumbai.

2. Reactions of 2-Chalcogenopyridine with palladium phosphine complexes, R. S. Chauhan, G. Kedarnath, A. M. Z. Slawin, V. K. Jain "3rd Asian Conference on Coordiantion Chemistry" 17-20 October 2011, Indian Habitate Centre, New Delhi.

3. Main group metal chalcogenolate complexes and their utility as molecular precursors for metal chalcogenides, R. K. Sharma, R. S. Chauhan, G. Kedarnath, A. Wadawale, V. K. Jain "National symposium on Frontier in Main-Group and Organometallic chemistry", 19- 20 December 2011, IISC, Bangalore.

4. Organometallic chemistry of platinum group metal chalcogenolates : Syntheis, Structures and Spectroscopy, R. S. Chauhan, G. Kedarnath, V. K. Jain "24th Research Scholar Meet-2012", 17-18 February, 2012, SIES College of Arts, Science and Commerce, Mumbai.

5. Organometallic chemistry of platinum group metal complexes derived from various hemilabile chalcogenolate ligands : Synthesis, spectroscopy and structures, R. S. Chauhan, G. Kedarnath, V. K. Jain "GECOM CONCOORD 2012" 3-8 June 2012, Metabief, France

Name : **Deepak Pandit**
Enrolment No. : PHYS04200804004
Constituent Institute : Variable Energy Cyclotron Centre, Kolkatta
Title : Study of High Energy Photons from Hot Nuclear Systems

Abstract

The high-energy photons from the decay of giant dipole resonance (GDR) have been used to study different reaction mechanisms at high excitation energy and angular momentum. The linearized GDR lineshapes for the system ^{47}V and ^{32}S populated via ^{20}Ne +^{27}Al and ^{20}Ne + ^{12}C, respectively, are remarkably different from each other. Interestingly, the two lineshapes are also dissimilar from what is observed for a spherical or a near spherical system indicating towards large deformations. The most striking feature for ^{47}V is the strong enhancement in the γ-ray yield at ~ 10 MeV. It is the characteristic of Jacobi shape transition, an abrupt change from an oblate to an elongated triaxial shape, and Coriolis effect due to high angular momentum. The experimental results are also consistent with the predictions of a hot rotating liquid drop model. However, no such enhancement is seen for ^{32}S nucleus although it is populated well beyond the Jacobi transition point. The shape looks more like a highly extended prolate and is seen for the first time for this nucleus. In this case, the thermal shape fluctuation model fails to explain the experimental data. The occurrence of such a large deformation without showing the characteristics of Jacobi transition is possible only if some other reaction mechanism is responsible. This unusual deformation has been speculated due to the formation of either the orbiting dinuclear configuration or the molecular structure of ^{16}O + ^{16}O forming a super-deformed structure in ^{32}S at high excitation.

Apart from the heavy-ion reaction, an extensive experiment was carried out to study the emission of high-energy photons from the spontaneous fission of ^{252}Cf source. Interestingly, high-energy γ-rays upto 80 MeV has ben observed in the experiment. The γ-rays in the range 8-20 MeV are attributed to the GDR γ-decay from the excited fission fragments while the spectrum about 20 MeV is attributed to the coherent bremsstrahlung due to the acceleration of the fission fragments in their mutual Coulomb field. The result has been substantiated with a theoretical calculation by estimating the emission of γ-rays considering classical Coulomb acceleration. This approximate calculation describes the experimental data remarkably well when the pre-scission kinetic energies of the fission fragments and the conservation of energy are taken into account.

Publications

1. "Critical behavior in the variation of GDR width at low temperature",Deepak Pandit, S. Mukhopadhyay, Surajit Pal, A. De and S. R. Banerjee, Phys. Lett. B713 (2012) 434.

2. "Measurement of giant dipole resonance width at low temperature: A new experimental perspective", S. Mukhopadhyay, Deepak Pandit, Surajit Pal, Srijit Bhattacharya, A. De, S. Bhattacharya, C. Bhattacharya, K. Banerjee, S. Kundu, T.K. Rana, G. Mukherjee, R. Pandey, M. Gohil, H. Pai, J.K. Meena , S.R. Banerjee, Phys. Lett. B 709 (2012) 9.

3. "Coherent bremsstrahlung and GDR width from 252Cf cold fission", DeepakPandit, S. Mukhopadhyay, Srijit Bhattacharya , Surajit Pal , A. De, S. R. Banerjee, Phys. Lett. B 690 (2010) 473.

4. "Extreme nuclear shapes examined via giant dipole resonance lineshapes in hot light-mass systems", Deepak Pandit, S. Mukhopadhyay,Srijit Bhattacharya, Surajit Pal, A. De,

S. Bhattacharya, C. Bhattacharya, K. Banerjee, S. Kundu, T. K. Rana, A. Dey, G. Mukherjee, T. Ghosh, D. Gupta, and S. R. Banerjee, Phys. Rev. C 81 (2010) 061302(Rapid).

5.   "A realistic technique for selection of angular momenta from hot nuclei: A case study with 4He + 115In → 119Sb* at ELab = 35 MeV", Deepak Pandit, S. Mukhopadhyay, Srijit Bhattacharya , Surajit Pal , A. De, S. R. Banerjee, NIM A 624 (2010) 148.

6.   "Variation of neutron detection characteristics with dimension of BC501A, neutron detector", K. Banerjee, T. K. Ghosh, S. Kundu, T. K. Rana, C. Bhattacharya, J. K.Meena, G.Mukherjee, P.Mali, D. Gupta, S.Mukhopadhyay, D Pandit, S. R. Banerjee, S.Bhattacharya , T. Bandyopadhyay, S.Chatterjee, NIM A 608 (2009) 440.

7.   "Giant dipole resonance width in nuclei near Sn at low temperature and high angular momentum", Srijit Bhattacharya, S. Mukhopadhyay, Deepak Pandit, Surajit Pal, A. De, S. Bhattacharya, C. Bhattacharya, K. Banerjee, S. Kundu, T. K. Rana, A. Dey, G. Mukherjee, T. Ghosh, D. Gupta, and S. R. Banerjee, Phys. Rev. C 77 (2008) 024318.

8.   "Scaling of the giant dipole resonance widths in hot rotating nuclei from the ground state values", Srijit Bhattacharya, Deepak Pandit, S.Mukhopadhyay, Surajit Pal, and S. R. Banerjee, Phys. Rev. C 78 (2008) 064601.

9.   "Consistency of nuclear thermometric measurements at moderate excitation", T. K. Rana, C. Bhattacharya, S. Kundu, K. Banerjee, S. Bhattacharya, A. Dey, T. K. Ghosh, G. Mukherjee, J. K. Meena,D. Gupta, S. Mukhopadhyay, D Pandit, S. R. Banerjee, A. Roy, and P. Dhara, Phys. Rev. C 78 (2008) 027602.

10.   "LAMBDA: Large Area Modular BaF2 Detector Array for the measurement of high energy gamma rays", S. Mukhopadhyay, Srijit Bhattacharya, Deepak Pandit, A. Ray, Surajit Pal, K. Banerjee, S. Kundu, T. K. Rana, S. Bhattacharya, C. Bhattacharya, A. De, S. R. Banerjee, NIM A 582 (2007) 603.

11.   "Characteristics of Gd-loaded liquid scintillators BC521 and BC525", K. Banerjee, S. Kundu, S. Mukhopadhyay, T.K. Rana, S. Bhattacharya, C. Bhattacharya, S. R. Banerjee, T.K. Ghosh, G. Mukherjee, T. Bandyopadhyay, A. Dey, J. K. Meena, P. Mukhopadhyay, D. Gupta, S. Pal, D Pandit, S. Bhattacharya, NIM A 580 (2007) 1383.

Name	:	**Yogesh Kumar Gupta**
Enrolment No.	:	PHYS01200804002
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Statistical and Dynamical Aspects in the Study of Compound Nucleus and Nuclear Fission

Abstract

This thesis work has been stimulated from the growing interest in exploring the exotic regions of the nuclear chart. Complete understanding of the diverse nuclear phenomena using the beams around the stability line of the nuclear chart, is a "stepping-stone" in the journey of nuclear chart exploration. Heavy-ion collisions provide an avenue to study the excited nuclei of a variety of choices in a wide range of excitation energy (E_x) and angular momentum (J). The present thesis, entitled with "Statistical and dynamical aspects in the study of compound nucleus and nuclear fissioin", is devided into parts: (i) the first part address the statistical aspects of the medium heavy compound nucleus, in particular the angular momentum dependence of the nuclear level density and (ii) second part addresses the dynamical aspects of the nuclear fission.

With the motivation of investigating the spin dependence of the nuclear level-density parameter 'a', a series of experiments were performed where we measured the γ-ray-multiplicity-fold gated α-particle energy spectra in heavy-ion fusion reactions which populate residual nuclei in the shell-closure region of Z~50 and mid-shell region of Z~70 at an excitation energy range of 30 to 40 MeV. The inverse level density parameter K (K=A/a) was determined by comparing the fold-gated as well as gross (summed overall J) experimental α-particle spectra with corresponding spectra from statistical model calculations using the code PACE2. The variation of K as a function of angular momentum in the range of 5 to 30ħ for the shell-closure region shows several interesting features. In contrast to the shell closure region of Z = 50, in the mid-shell region of Z~70 the average value of K is 8.2± 1.1 MeV, and remains essentially constant around the average value. These are new experimental findings which provide crucial input to test the microscopic therories.

In the second part of my thesis, we investigated the charged particle accompanied fission in a wide energy range from low energy fission to heavy-ion induced fission. The charged particle emission during the fission takes place from various stages of the fission process. Particularly, the α-particle emission near the neck region (ternary fission) has been in dispute in terms of emission mechanism whether it is a statistical or dynamical in nature. It has been unambiguously revealed that the ternary emission of α particules in heavy-ion induced fisson is statistical in nature whereas it is purely a dynamical one for spontaneous and neutron induced fission. It indicates that the neck collapse is faster in low energy or spontaneous fisson whereas at higher excitation energy it is slow process. It is, therefore, inferred that the nuclear collective motion during the scission exhibits a change over from super fluid to viscous behavior with increasing excitation energy. In one of the measurements we have identified a new source of α-particle emission in $^{12}C+^{232}Th$ fission which has been attributed to the transfer-breakup process.

This work also includes nuclear instrumentation development work. Various innovative methods of using (CsI(TI)-Si(PIN) and gas ionization chambers has been demonstrated.

Present thesis work led to five publications in international peer reviewed journals, and invites many new experimental and theoretical investigations.

Publications

1. *Tellurium*(0) as a ligand: Synthesis and characterization of 2-pyridyltellurolates of platinum II) and structures of [Pt{2-Te-3-(R)C H N Te(PR')}] (R = H or Me). R. S. Chauhan, G. Kedarnath, A. Wadawale, A. M. Castro, R. A. Perez, V. K. Jain, W. Kaim *Inorg. Chem* 49 (2010) 4179-4185.

2. Reactions of 2-tellur opyridine ligands with (diphosphine)P and (diphosphine)PtCl 2 complexes and isolation of different structural motifs of platinum(II)complexes. R. S. Chauhan, G. Kedarnath, A. Wadawale, A. L. Rheingold, A. M.Castro, R. A, Perez, V. K. Jain *Organometallic* s, 31, 2012) 1743-17504

3. Reactivity of dipyrimidyldiselenides with [M(PPh3) 4 and 2-pyrimidylchalcogenolates with [MCl2 (diphosphine)] (M = Pd or Pt) R. S. Chauhan, R. K. Sharma, G. Kedarnath, D. B. Cordes, A. M. Z. Slawin, V. K. Jain *J. Organomet. Chem.* 717 (2012) 180-186.

4. Reactivity of 2-chalcogenopyridines with palladium-phosphine complexes: Isolation of different complexes depending on the nature of chalcogen atom R. S. Chauhan, G. Kedarnath, A. Wadawale, A. M. Z. Slawin, V. K. Jain *Dalton Trans.,* 42 (2013) 259-269.

5. Oxidative addition reactions of nicotinamide based organoselenium compounds on [M(PPh3) 4] (M = Pd or Pt) : An insight study for the formation of several isolable products R. S. Chauhan, C. P. Prabhu, P. P. Phandis, G. Kedarnath, J. A. Golen, A. L., Rheingold, V. K. Jain *J. Organomet. Chem.* , 723 (2013) 163-170.

6. Bis phosphine palladium(II) mesityl chalcogenolate complexes: Synthesis and structure of [Pd(SeMes)2(dppe)] R. S. Chauhan, G. Kedarnath, A. Wadawale, J. A. Golen, A. L. Rheingold, V. K. Jain, *Ind. J. Chem.,* 52 A (2013) 42-44.

7. Bis phosphine palladium(II) mesityl chalcogenolate complexes: Synthesis and structure of [Pd(SeMes)2(dppe)] R. S. Chauhan, G. Kedarnath, A. Wadawale, J. A. Golen, A. L. Rheingold, V. K. Jain *Ind. J. Chem.,* 52 A (2013) 42-44.

8. Cis configured bis phosphine platinum(II) chalcogenolate complexes: Structures and a comparative NMR study R. S. Chauhan, G. Kedarnath, A. Wadawale, J. A. Golen, A. L. Rheingold, V. K. Jain *J. Organomet. Chem.* (submitted)

Conferences/Symposia

1. Structural and spectroscopic characterization of platinum complex with C-substituted (pyridyltelluro)-bis(diphenylphosphino)methane, R. S. Chauhan, G. Kedarnath, A. Wadawale, V. K. Jain "3rd International Conference on Materials Chemistry", 7-10 December 2010, BARC, Mumbai.

2. Reactions of 2-Chalcogenopyridine with palladium phosphine complexes, R. S. Chauhan, G. Kedarnath, A. M. Z. Slawin, V. K. Jain 3rd Asian Conference on Coordiantion Chemistry" 17-20 October 2011, India Habitate Centre, New Delhi. "3rd International Conference on Materials Chemistry", 7-10 December 2010, BARC, Mumbai.

3. Main group metal chalcogenolate complexes and their utility as molecular precursors for metal chalcogenides, R. K. Sharma, R. S. Chauhan, G. Kedarnath, A. Wadawale, V. K. Jain "National symposium on Frontier in Main-Group and Organometallic chemistry", 19-20 December 2011, IISC, Bangalore.

4. Organometallic chemistry of platinum group metal chalcogenolates : Syntheis, Structures and Spectroscopy, R. S. Chauhan , G. Kedarnath, V. K. Jain "24th Research Scholar Meet-2012", 17-18 February, 2012, SIES College of Arts, Science and Commerce, Mumbai.

5. Organometallic chemistry of platinum group metal complexes derived from various hemilabile chalcogenolate ligands : Synthesis, spectroscopy and structures R. S. Chauhan, G. Kedarnath, V. K. Jain GECOM CONCOORD 2012" 3-8 June 2012, Metabief, France

Name	:	**Seemita Banerjee**
Enrolment No.	:	CHEM01200804001
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Statistical and Dynamical Aspects in the Study of Compound Nucleus and Nuclear Fission

Abstract

In recent years, research in materials science has shown a rapid expansion towarddiscoveries of suitable materials for sustainable energy. A hydrogen economy is proposed tosolve the ill effects of using hydrocarbon fuels in transportation and other end-use applications, where carbon is released to the atmosphere. In this context the storage of hydrogen poses the biggest challenge in a new hydrogen economy, because the storage medium must meet the requirements of high gravimetric and volumetric density, fast kinetics and favorable thermodynamics.

The Main focus of this thesis is towards developing new hydrogen storage materials from application perspectives. Transition metal based alloys, viz. Ti-V-Fe, Ti-V-Cr and Zr-Fe-V, have been investigated in detail to find the prospect of appropriate doping in these alloy system to obtain potential future storage matrices with higher hydrogen loading capacity and favorable absorption desorption kinetics. The alloys were synthesized by controlled atmosphere are melting and characterized for structure and morphology by XRD, SEM/EDAX, EPMA. The hydrogen storage properties of these oxides were evaluated in an indigenously developed volumetric Sievert's type set up. The structural variations of the alloys and their hydrides with different types and levels of doping were found to be useful in correlating the structure property relationship. Further, the desorption behavior of the hydrides evaluated both in-situ and with air exposed samples by TPD, DSC, TG and DTA.

In the thesis the Mg and C based system was investigated for hydrogen storage using first principle calculations. For Mg based systems the results have indicated the relative stabilities of Mg(0001) surfaces doped with different transition metal atoms, substituted on substituted layers of atoms. Also the interaction energies of hydrogen with differently substituted Mg (0001) surface have been calculated and the activation barrier for the dissociation and diffusion of hydrogen goves clear idea about the choice of doping elements for developing Mg based hydrogen storage materials. The representative studies on carbon based materials namely; SiC nano materials, doped corannulene and metallo-carbohedrene for their hydrogen absorption properties have revealed possible compositions and structural configurations that show promising hydrogen storage characteristics.

Publications

1.   Seemita Basak, K. Shashikala, P. Sengupta, S. K. Kulshreshtha, "Hydrogenabsorption properties of Ti–V–Fe   alloys: Effect of Cr substitution", *International Journal of Hydrogen Energy,* 32, 4973, (2007).

2.   Seemita Basak, K. Shashikala, S.K. Kulshreshtha, "Hydrogen absorption characteristics of Zr substituted Ti0.85VFe0.15 alloy", *International Journal of Hydrogen Energy,* 33, 350, (2008).

3.   K. Shashikala, Seemita Banerjee, Asheesh Kumar, M. R. Pai and C. G. S. Pillai; "Improvement of hydrogen storage properties of TiCrV alloy by Zr substitution for Ti", *International Journal of Hydrogen Energy,* 34, 6684, (2009)

4. Seemita Banerjee, C. G. S. Pillai, and C. Majumder, "First-principles study of the H2 interaction with transition metal (Ti, V, Ni) doped Mg(0001) surface: Implications for H-storage materials" *Journal of Chemical Physics,* 129, 174703 (2008).

5. Seemita Banerjee, C. G. S. Pillai, and C. Majumder; "Dissociation and Diffusion of Hydrogen on the Mg(0001) Surface: Catalytic Effect of V and Ni Double Substitution", *Journal of Physical Chemistry C,* 113, 10574, (2009).

6. Seemita Banerjee, C. G. S. Pillai, C. Majumder, "Adsorption and desorption of hydrogen in Mg nanoclusters: Combined effects of size and Ti doping", *International Journal of Hydrogen Energy,* 35, 2344, (2010).

7. Seemita Banerjee, C. G. S. Pillai, C. Majumder, "Hydrogen absorption behavior of doped corannulene: A first principles study" *International Journal of Hydrogen Energy,* 36, 4976 (2011). 332

8. Asheesh Kumar, K. Shashikala, Seemita Banerjee, J Nuwad, Priyanka Das, C. G. S. Pillai, "Effect of cycling on hydrogen storage properties of Ti2CrV alloy" *International Journal of Hydrogen Energy,* 37, 3677 (2012).

9. S. Banerjee, Sandeep Nigam, C. G. S. Pillai, C. Majumder, "Hydrogen Storage on Ti Decorated SiC Nanostructures: A First Principles Study", *International Journal of Hydrogen Energy*, 37, 3733 (2012).

10. K. Shashikala, Asheesh Kumar, C. A. Betty, Seemita Banerjee, P. Sengupta and C.G. S. Pillai, "Improvement of the hydrogen storage properties and electrochemicalcharacteristics of Ti0.85VFe0.15 alloy by Ce substitution", *Journal of alloys and compounds*, 509, 9079 (2011).

11. Seemita Banerjee, C. G. S. Pillai, C. Majumder, "High capacity reversible hydrogen storage by metallo-carbohedrenes: An ab initio molecular dynamic simulation study" *Applied Physics Letters*, Available online DOI: 10.1063/1.4792686.

Name	:	**Manoj Kumar Sharma**
Enrolment No.	:	CHEM01200604032
Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Synthesis, Characterization and Electrochemical Applications of Nanomaterials

Abstract

In the present thesis entitled "Synthesis, Characterisation and Electrochemical Applications of Nanomaterials", nanomaterials of noble metal (Au and Pt) were prepared and the electrochemical behavior of the actinides (uranium and plutonium) was studied on the nanomaterial- modified electrodes.

An in situ one step chemical synthesis of gold-polyaniline composite was carried out in track-etched polycarbonate membrane and gold-polyaniline composite was characterized. Nanopores in the polycarbonate membrane act as the reactin vessels of nano-dimension whrer aniline and HA_uCl_4 were allowed to mix together and the redox reaction between aniline and HA_uCl_4 led to the synthesis of gold-polyaniline composite. The nanopores also controlled the growth of gold-polyaniline composites by limiting the free volume available for the growth. Track-etched polycarbonate membrane acted as a supporting matrix for immobilization of gold-polyaniline composites.

Mercury was used a cathode material for the electrochemical template synthesis of gold nanorods within the pores of track-etched PC membrane. This new approach eliminates the requirement of coating a 500 nm to 1 µm thick metallic layer (working as cathode) onto one surface of an insulating membrane by sputter deposition technique. A simple two-compartment electrochemical cell was used and the track-etched polycarbonate membrane was placed between the two compartments separating the aqueous solution of HA_uCl_4 from mercury. Mercury, filled in one of the compartment, was in contact with one surface of the membrane (similar to sputter deposited metallic layer) and served as the conducting substrate/cathode. The ensemble of the metal nanowires grown in the template membrane was not attached to any conducting substrate, and gold nanorods could be easily freed from the template membrane after dissolution in dichloromethane.

Pt nanoparticles (PtNPs) were electrochemically deposited on the surface of Pt and glassy carbon electrodes. The electrochemical behavior of Pu(IV)/Pu(III) redox couple in 1 M H_2SO_4 was studied on PtNPs-modified electrode and compared to that of the bare electrodes. Redox kinetics improved in both the oxidation and the reduction processes after electrodeposition of PtNPs in contrast to bare electrodes. However, significatnt improvement was seen for the reduction of Pu(IV) to Pu(III) in PtNPs-coated GC electrode compared to the bare GC electrode. These studies are of great relevance to develop electroanalytical methodologies ofr Pu determination using nanoparticles modified electrodes.

Electrochemical behavior of UO_2^{2+} ions was studied at gold nanoparticles-modified electrodes. The modified electrodes were prepared by either physical entrapment of gold nanoparticles (AuNPs) in an anion-exchange membrane or by formation of gold nanoporous film (AuNPF) on bare Au electrode.

Gold nanoparticles (AuNPs) were synthesis in the matrix of a cellulose triacetate (CTA) membrane containing an anion-exchanger (Aliquat 336), and AuNPs-CTA membrane was used to modify the gold electrode. Cycle voltammetric and impedance studies were carried out to see the effect of nanoparticles modified electrode on the partial electrochemical irreversibility of the carbonato-complexes of U(VI)/U(V). Electrochemical studies showed the electrocatalytic reduction of UO_2^{2+} to UO_2^+ in saturated Na_2CO_3 solution at AuNps-CTA modified electrode with higher current density and faster

heterogeneous electron transfer kinetics (smaller ($\triangle$Ep) than that using bare Au electrode. The standard heterogeneous rate constant, $K^{0,}$ for the reduction precess at AuNPs-CTA modified electrode was about 25 times higher than that of bare Au electrode. Therefore, it was concluded that AuNPs-CTA membrane significantly improved the interfacial electron-transfer properties, resulting in a better electrochemical response than bare Au electrode.

Gold nanoporous film (AuNPF) was grown on bare gold electrode by electrochemical oxidation and electrochemical reduction of UO_2^{2+} in 0.5 M H_2SO_4 was studied on AuNPF electrode. In cyclic voltammetric (CV) studies, anodic shift of 141 mV in the cathodic peak potential and an increase in the reduction current was observed at the AuNPF electrode, showing evidence of its enhanced electrochemical activity as compared to that of the bare Au electrode. The interrfacial charge transfer resistance values for the bare Au and the AuNPF electrodes. The chronomperometric studies indicated the thin-layer diffusion within the gold nanoporous film. Therefore, the observed anodic shift at the AuNPF electrode was attributed to the contribution from thin-layer diffusion within the gold nanoporous film.

Publications

1.   Seemita Basak, K. Shashikala, P. Sengupta, S. K. Kulshreshtha, "Hydrogen absorption properties of Ti–V–Fe alloys: Effect of Cr substitution", *International Journal of Hydrogen Energy,* 32, 4973, (2007).

2.   Seemita Basak, K. Shashikala, S.K. Kulshreshtha, "Hydrogen absorption characteristics of Zr substituted Ti0.85VFe0.15 alloy", *International Journal of Hydrogen Energy,* 33, 350, (2008)

3.   K. Shashikala, Seemita Banerjee, Asheesh Kumar, M. R. Pai and C. G. S. Pillai; "Improvement of hydrogen storage properties of TiCrV alloy by Zr substitution for Ti", *International Journal of Hydrogen Energy,* 34, 6684, (2009).

4.   Seemita Banerjee, C. G. S. Pillai, and C. Majumder, "First-principles study of the H2 minteraction with transition metal (Ti, V, Ni) doped Mg(0001) surface: Implications for H-storage materials" *Journal of Chemical Physics,* 129, 174703 (2008).

5.   Seemita Banerjee, C. G. S. Pillai, and C. Majumder; "Dissociation and Diffusion of Hydrogen on the Mg(0001) Surface: Catalytic Effect of V and Ni Double Substitution", *Journal of Physical Chemistry C,* 113, 10574, (2009).

6.   Seemita Banerjee, C. G. S. Pillai, C. Majumder, "Adsorption and desorption of hydrogen in Mg nanoclusters: Combined effects of size and Ti doping", *International Journal of Hydrogen Energy,* 35, 2344, (2010).

7.   Seemita Banerjee, C. G. S. Pillai, C. Majumder, "Hydrogen absorption behavior of doped corannulene: A first principles study" *International Journal of Hydrogen mEnergy,* 36, 4976 (2011).332

8.   Asheesh Kumar, K. Shashikala, Seemita Banerjee, J Nuwad, Priyanka Das, C. G. S. Pillai, "Effect of cycling on hydrogen storage properties of Ti2CrV alloy" *International Journal of Hydrogen Energy,* 37, 3677 (2012).

9.   S. Banerjee, Sandeep Nigam, C. G. S. Pillai, C. Majumder, "Hydrogen Storage on Ti Decorated SiC Nanostructures: A First Principles Study", *International Journal of Hydrogen Energy*, 37, 3733 (2012).

10.   K. Shashikala, Asheesh Kumar, C. A. Betty, Seemita Banerjee, P. Sengupta and C. G. S. Pillai, "Improvement of the hydrogen storage properties and electrochemical characteristics of Ti0.85VFe0.15 alloy by Ce substitution", *Journal of alloys and compounds*, 509, 9079 (2011).

11.   Seemita Banerjee, C. G. S. Pillai, C. Majumder, "High capacity reversible hydrogen storage by metallo-carbohedrenes: An ab initio molecular dynamic simulation study" *Applied Physics Letters*, Available online DOI: 10.1063/1.4792686.

Name	:	**Ms. Poulami Das**
Enrolment No.	:	LIFE09200604005
Constituent Institute	:	Tata Memorial Centre, Mumbai
Title	:	Identification of Specific Genetic Alterations in Cervical Cancer by Genome Wide LOH and Copy Number Analysis

Abstract

With about 134000 new cases and 72800 deaths annually, cancer of the uterine cervix accounts for the most frequent cancer among women in India. Although HPV infection has been shown to play a critical role in the aetiology of cervical cancer, genetic alterations also contributes significantly to the pathogenesis of the disease. The main focus of the study was to understand the role of HPV infection and genetic alterations in a cohort of Indian women with locally advanced cervical carcinoma.

The incidence of HPV as well as different genotypes was determined in 270 pretreatment cervical cancer biopsies using PCR with 3 different primer sets and high-throughput luminex bead array. The overall HPV positivity was 95% and the incidence of HPV16 and/or HPV18 was the highest (72%). We then determined the physical state of the virus as well site of viral integration was in a subset of cases (n=86) positive for HPV16 and/or HPV18 by APOT assay. Integration was observed in 79% cases and was found to be more frequent at chromosomal loci 1p, 3q, 13q, 6q, 11q and 20q. Also, protein coding genes as well as fragile sites were identified as potential hotspots. Comparison with clinical outcome revealed that patients with only episomal form of HPV had a better disease free survival as compared to those with integrated form. We also determined the viral load in the same 86 cases with known physical status by SYBR green based quantitative real time PCR. It was observed that high viral load combined with integration served as a worst prognostic marker.

In order to understand the genetic alterations in the tumour samples, whole exome sequencing of 11 cervical biopsies and 8 matched controls (blood from the same patients) was done. A number of interesting germline (such as RNASEL, PTPRJ, ZFP64, etc.) and somatic (FGF7, SOS2, DIDO1 and MAP3K3, RASA1, etc.) variations were identified and further validated by Sanger sequencing. These might represent predisposing and/ or potential disease causing mutations. The data, besides being a source of information on novel variations in the Indian genome (which the dbSNP currently lacks), would mark the beginning of understanding the genomic landscape of cervical cancer.

The significance of the study lies in the fact that we have addressed all the major factors associated with pathogenesis of cervical cancer and assessed the role of each. The genetic analysis of the next generation data would be firs of its kind on Indian cervical cancer patients. Such approaches would help in better understanding the fundamental rules of cervical carcinogenesis and be a step forward towards identifying biomarkers and newer treatment modalities for management and cure of the disease.

Publications

1. Poulami Das, Asha Thomas, Umesh Mahantshetty, Shyam K., Srivastava, Kedar Deodhar, Rita Mulherkar HPV genotyping and site of viral integration in cervical cancers in Indian Women. PLoS ONE (PONE-D-12/05501R1)

Name   :   **Niharika Singh**

Enrolment No.   :   PHYS01200704030

Constituent Institute   :   Bhabha Atpmic Research Centre, Mumbai

Title   :   Studies in Coherent Pump-Probe Spectroscopy of Three and Four Level Systems

Abstract

Manipulation and control of atomic response by electromagnetic fields is one of the central themes of quantum optics research in recent years. These control strategies rely on quantum coherence and interference, and their manifestations in driven multi-level atomic/molecular systems. This thesis embodies studies of quantum interference and associated phenomena in coherently driven three- and four-level systems with the objective of achieving control of interaction between atomic/molecular systems and electromagnetic fields. The specific issues addressed are electromagnetically induced transparency (EIT), electromagnetically induced absorption (EIA), amplification without inversion (AWI), spontaneously generated coherence (SGC), Kerr nonlinearity and the effect of laser phase fluctuations. Also examined are the issues related to the effect of permanent dipole moments on the coherent dynamics of molecular systems, subluminal and superluminal light propagation and realization of negative refractive index in coherently prepared atomic medium. These phenomena help to understand the subtle quantum effects in laser-atom interactions, they on the other hand provide useful platform for development of quantum technologies. The major part of the thesis concentrates on the theoretical development of light-matter interaction and analysis of the aforementioned effect. These studies have been done in the framework of master equation and quantum jump approach, and the systems investigated are three-and four-level atoms/molecules in various level configurations, i.e., Λ, double Λ, tripod, Nresonance etc [10]. In order to provide a flavor of coherent pump-probe spectroscopy for precision measurements, few experimental results are also reported for a medium of alkali atoms. The work reported in the thesis thus provides avenues for newer studies in the field of quantum optics.

Publications

Journal Publications

a. Published

1. Sub-natural linewidth resonances in coherently-driven double Λ system. Niharika Singh, Q.V. Lawande, R. D'Souza and B.N. Jagatap, Pramana- J. of Phys. 75, 1151 (2010).

2. Resonances in the pump-probe spectroscopy of Λ system in alkali atoms. Niharika Singh, Y.B. Kale, A. Ray and B.N. Jagatap, Indian J. Phys. 84, 1119 (2010).

3. Modulation transfer in Doppler broadened Λ system and its application to frequency offset locking. Y.B. Kale, A. Ray, Niharika Singh, Q.V. Lawande and B.N. Jagatap, Eur. Phys. J. D. 61, 221 (2011).

4. Coherent pump-probe spectroscopy of four level atomic systems. Niharika Singh and B.N. Jagatap, AIP Conf. Proc. 1391, 16 (2011).

5. Double control electromagnetically induced transparency windows in a tripod system. Niharika Singh, R. D'Souza, Q.V. Lawande and B.N. Jagatap, Asian Journal of Physics, 20, 221 (2011). *Synopsis*

6.   Electromagnetically induced transparency in a Λ-type molecular system with ermanent dipole moments revisited. Niharika Singh, Q.V. Lawande, R. D'Souza and B.N. Jagatap, J. Chem. Phys. 137, 104309 (2012).

b. Communicated

1.   Coherent pump-probe spectroscopy of a Λ system with a close lying excited level. Niharika Singh, A. Ray, R. D'Souza, Q.V. Lawande and B.N. Jagatap.

2.   Amplification without inversion in a four level atomic system in degenerate double Λ configuration. Niharika Singh, R. D'Souza, Q.V. Lawande and B.N. Jagatap.

3.   Laser phase fluctuations in a four-level atomic system in N-configuration.Niharika Singh, R. D'Souza, Q.V. Lawande and B.N. Jagatap.

II. Books/Reports/General Articles

1.   Ultrasensitive Magnetometry: Exploring Ultra-low Magnetic Fields in the Physical World. Niharika Singh, A. Ray and B.N. Jagatap, IWSA Newsletter, p.13 (2010).

2.   Spectroscopy of coherently prepared three and four level medium. Niharika Singh, A. Ray, Y.B. Kale and B.N. Jagatap , Emerging Trends in Laser and Spectroscopy and Applications, published by Allied Publishers Private Limited, New Delhi, p.261 (2010).

3.   Spectroscopy in coherently prepared atomic medium and its applications. Y.B. Kale, Niharika Singh, A. Ray and B.N. Jagatap, Kiran, Vol. 21, 2, p.22 (2010). *Synopsis*

4.   Precision spectroscopy of coherently prepared three and four level atomic medium. Niharika Singh, A. Ray, Y.B. Kale and B.N. Jagatap, BARC Newsletter, Founder's day special issue, p.271 (2010).

5.   Electromagnetically induced transparency in a tripod atomic system. Niharika Singh, Q.V. Lawande, R. D'Souza and B.N. Jagatap, Kiran, vol. 22, 1, p.21 (2011).

6.   Electromagnetically induced transparency in a tripod atomic system. Niharika Singh, R. D'Souza, Q.V. Lawande, and B.N. Jagatap, BARC Newsletter, Founder's day special issue, p.382 (2011).

III. Conferences/Symposia

1.   Amplification without inversion in a degenerate double lambda system. Niharika Singh, R. D'Souza, Q.V. Lawande and B.N. Jagatap, IEEE Conference Series, Conference on lasers and electro optics (CLEO) technical digest, Optical Society of America, art. no. 6326327, p. JTh2A.35 (May 6-11, 2012).

2.   Coherence induced negative refractive index in a 4 level atomic medium. Niharika Singh, Q.V. Lawande, R. D'Souza and B.N. Jagatap, Proceedings of International Conference on Quantum Optics and Quantum Computing (ICQOQC- 2011), Department of Physics and Materials Science and Engineering, Jaypee Institute of Information Technology, Noida, p.70 (March 24-26, 2011).

3.   Spectroscopy in coherent atomic medium. Niharika Singh, A. Ray, Y.B. Kale and B.N. Jagatap, Proceedings of Meghnad Saha Memorial Symposium on Emerging Trends in Laser & Spectroscopy and *Synopsis* Applications (MMSETLSA-2009), University of Allahabad, (March 23-25, 2009). (Best poster award).

4.   Sub-natural linewidth resonances in coherently driven double Λ system. Niharika Singh, Q.V. Lawande, R. D'Souza, A. Ray and B.N. Jagatap, Proceedings of National Laser Symposium (NLS-09), Bhabha Atomic Research Centre, Mumbai, p.68 (January 13-16, 2010).

5.   Electromagnetically induced transparency in four and five level atomic systems. Niharika Singh, Q.V. Lawande, B.N. Jagatap and R. D'Souza, Proceedings of Topical Conference on Interaction of

EM Radiation with Atoms, Molecules and Cluster (TC-2010), Raja Ramanna Centre for Advanced Technology, Indore, p.72 (March 03–06, 2010).

6. Electromagnetically induced transparency in a tripod atomic system. Niharika Singh, Q.V. Lawande, R. D'Souza and B.N. Jagatap, Proceedings of National Laser Symposium (NLS-19), Raja Ramanna Centre for Advanced Technology, Indore, p.75 (December 1-4, 2010). (Best poster award).

7. Realization of negative refractive index: Theoretical analysis for a coherently driven four-level system. Niharika Singh, R. D'Souza, Q.V. Lawande and B.N. Jagatap, Proceedings of National Laser Symposium (NLS-19), Raja Ramanna Centre for Advanced Technology, Indore, p.76 (December 1-4, 2010).

8. Amplification without inversion in degenerate and non-degenerate double lambda system.

Annex 6

Titles of M.Tech, M.Phil & M.Sc. (Engg.) theses for which results were notified during April 1, 2012 to March 31, 2013

Titles of M.Tech. Theses for which results were notified
during April 1, 2012 to March 31, 2013

SL. No.	Name of the Student	Date of Notification of degree	Thesis Title
1.	Shri Y. Prashant	17.04.12	Controlling Bio-fouling and Microbiologically Induced Corrosion(MIC) of Nuclear and Marine Condenser Materials through Surface Modification
2.	Ms. Madhusmita Baral	17.04.12	Investigation of the Electronic Structure of Ferromagnetic Heusler Alloys by Photoelectron Spectroscopy(PES)
3.	Shri Arvindkumar Singh	17.04.12	Development of a Simulator for Sodium Iodide[NaI(Tl)] Scintillator Detector alongwith a Simulator for Cs-137 Source
4.	Shri Ashok Kumar	17.04.12	Preparation and Structural Characterization of Some Pb based Relaxor Ferroelectrics
5.	Shri Anand Venkataramakrishnan	17.04.12	Design and Development of Universal Remote Terminal Units using FPGAs for Control Applications in FBRs
6.	Shri Sanjeev Kumar Poudel	17.04.12	A Novel Baseline Restorer cum Peak Stretcher Circuit based Design of Position Encoding Electronics for Neutron Position Sensitive Detectors
7.	Shri Ravi Sharma	17.04.12	Development of Laser based Remote Vibration Measuring Device
8.	Ms. Gita S. Kumar	17.04.12	Study and Development of Uniform Communication Mechanism for Multifunction CPU Board
9.	Shri Suvadip Pal	17.04.12	Design of Adaptive Controller for Electron Beam Evaporation System
10.	Shri Vikas Kumar Sahu	17.04.12	Studies on Structural, Optical and Electrical Properties of ZnO Thin Films Grown using Layer Deposition

11.	Shri Surojit Saha(BARCTS, Mumbai)	17.04.12	Comparative Study and Experimental Evaluation of Localisation Methods for Mobile Robots in Indoor Environments
12.	Shri Vinay Kumar Srivastava	17.04.12	Experimental Studies and Analytical Modeling of TPB Specimens under Dynamic Loading
13.	Shri Alok Kumar	17.04.12	Experimental Evaluation of Material Flow for 6061 T6 Aluminium at Elevated Strain Rates and Temperature and its Application in FE Analysis
14.	Ms. Lovely Paliwal	17.04.12	Development of Automated TL-OSL Reader System for Radiation Dosimeters & Environmental Monitoring Applications
15.	Shri Ritesh Raj	17.04.12	Assessment of Hydrogen Generation and Simulation of Thermal Hydraulic Scenario & Sequences of Event Involving Postulated Beyond Design Basis Accident for TAPS- 1 & 2 using SCDAP/ RELAP- 5/MOD- 3.2 Code
16.	Shri Sandeep Gaur	17.04.12	Development of Tuned Liquid Damper with Semi Active Gel
17.	Shri Anurag Sawhney	17.04.12	Study, Analysis and Development of Neutron-Gamma Discrimination Techniques for Plastic Scintillators using Digital Signal Processing
18.	Shri Ankit Pilania	17.05.12	Determination of Source Term in Subcritical Reactor by Noise Analysis Technique
19.	Shri Abhishek Jain(BARCTS, Kalpakkam)	17.05.12	Development of Cavity Support System for Cryomodule of 650 MHz SCRF Cavities
20.	Shri Nitin Nigam(BARCTS, Mumbai)	17.05.12	Optimization of Design and Lorentz Force Tuning Methodology for Superconducting Radio Frequency Cavity for Charged Particle Accelerator
21.	Ms. Samyuktha Gaddam	18.05.12	Recovery of Lithium from Simulated Spent Lithium Titanate Pebbles
22.	Shri Vijay Suresh Mamtani	18.05.12	Fouling Studies of Capillary Ultrafiltration(UF) Membranes
23.	Ms. Sonali Parashar(BARCTS, Indore)	18.05.12	Simulation and Modelling of Beam Dynamics of 10 MeV, 10 kW RF Linac

24.	Shri Aritra Sarkar	18.05.12	Deformation Behaviour under Ratcheting of a Type 316LN Stainless Steel
25.	Ms. Payal Singhai(BARCTS, Indore)	18.05.12	A Study of Radiation Pulse Processing Techniques and its Implementation on FPGA
26.	Shri Mahesh Punna	22.05.12	Functional Programming Methodology for the Design of Gamma Spectral Analysis Package
27.	Shri Manisankar Dhabal	31.05.12	Design and Development of Advanced Embedded Data Acquisition System for Remote Sensors
28.	Ms. Monali Kulkarni	31.05.12	Development and Evaluation of a Document Clustering Engine
29.	Shri Navtesh Bajpai	15.06.12	Application of Advanced UT on Corner Weld Joints of Jacketed Annular Tanks
30.	Shri Rupesh Patel	15.06.12	Design, Development and Analysis of 10 kHz, 10 kW Solid State Inverter for DC Accelerator Applications
31.	Shri Dnyaneshwar Laxman Awasare(BARCTS, Tarapur)	15.06.12	Studies on Biocidal Efficiency of Chlorine Dioxide on Sea Water used as Coolant for Power Plants and Process Industries
32.	Ms. Rita Behera(BARCTS, Indore)	15.06.12	Study and Generation of Ultra Narrow Resonance Arising from Quantum Interference
33.	Shri Vikram Sekar	27.06.12	Study of C&I Cable Failure and Evaluation of Techniques for Insulation Resistance Measurement
34.	Shri Govardhan Prasad P.	27.06.12	Experimental and Numerical Investigation of High Velocity Impact on Aluminium Alloy Plate
35.	Shri Arun Pooleery	27.06.12	Optimisation of Rolled Joint End Fitting and Pressure Tube of 700 MWe PHWR
36.	Shri Vikas Rakshit(NTC, Kalpakkam)	27.06.12	Algorithm Development for Automated Wavelength Control of SLM Dye Lasers
37.	Ms. Sowmya K.	04.07.12	Study of Heat Transfer Characteristics in an Inclined Rotary Evaporator
38.	Shri Saurabh Mishra(BARCTS, Indore)	04.07.12	Volumetric Control and Machine Vision of Falling Antibodies/DNA Spots
39.	Shri Ram Kumar Paul	04.07.12	Design and Analysis of the Control System of High Voltage (400 kV, DC) Power Supply for Neutron Generator

40.	Shri M. Nimala Sundaran	04.07.12	Testing and Evaluation of Natural Vibration Behaviour of CSRDM with Control SubAssembly
41.	Shri Nirvik Sen	18.07.12	Study on Hydrodynamic Dispersion in Compact Geometries of Tubes
42.	Shri Sarthak Gupta(BARCTS, Mumbai)	07.08.12	Performance Evaluation of Computing Clusters for Improved QoS
43.	Lt. Cmdr. Dinku Borah	07.08.12	Establishing the Role of Alloying Additions in Austenitic Stainless Steels on Susceptibility to IGC and IGSCC Through Time-Temperature-Sensitization Diagrams
44.	Lt. Col. Saumitra Mohan Joshi	07.08.12	Development of Electrochemical Test to Detect Phosphorous Segregation in Cr-Mo Steels
45.	Shri Prince Kumar Jain	07.08.12	Modeling of Transient Flows in the Experimental Lead Bismuth Eutectic(LBE) Neutron Target for ADS
46.	Ms. Pragati Shukla	07.08.12	Modeling and Simulation of Electrolyser with Flowing Mercury Electrode
47.	Lt. Cdr. Rohit Kumar	07.08.12	Development of Synchronization System for Two Spark Gaps
48.	Shri Aniruddha Ghosh	07.08.12	Online Prognostics and Health Monitoring of Swing Type Check Valves
49.	Lt. Cdr. Jayanth Vaithianathan	10.08.12	Seismic Response Control of Structures using Semi Active Tuned Liquid Damper With Ferrofluid
50.	Wg. Cdr. Ajit Kumar Sinha	10.08.12	Development of a Simplified Methodology for Analysing Piping System Suported on Visco-Elastic Damper
51.	Ms. Krishna Rathore	10.08.12	Nuclear Data Assimilation and Analysis Using Kalman Filter for Radiation Monitoring
52.	Maj. Rajesh Dwivedi	16.08.12	Design and Development of Pulse Modulator
53.	Shri Ankur Agrawal	18.08.12	Design and Development of Online Flux Monitoring System for INDUS- 1 Beam-Line to Compensate EMI Emerging from Various Sources
54.	Shri Ratheesh Kumar N. S.	18.08.12	Stress Corrosion Cracking of Austenitic Stainless Steels in Chroride Environment: Effet of Surface Finish, Temperatute and Chloride Concentration on SCC Initiation
55.	Lt. Cdr. Vinamra Mishra	18.08.12	Analytical Modeling of Reactor Regulating System of Light Water Reactors

56.	Shri Sayan Dey Chaudhuri	18.08.12	Non-Destructive Technique for Measurement of Helium Gas Pressure Inside PFBR Fuel Pins
57.	Lt. Cdr. Chirag Verma	18.08.12	Parametric Study and Process Control of Electron Beam Physical Vapour Deposition System for High Reflective Coating
58.	Ms. Jinimol Joy	20.08.12	Copper Electrodeposition to Simulate Electrorefining for Pyroprocessing
59.	Shri V. Sudharshan	20.08.12	Process Design of Intermediate Heat Exchanger for Future 500 Mwe Fast Breeder Reactors
60.	Shri Balla Sai Prasad(NTC, Tarapur)	25.08.12	Degradation Modes of Alloy 600 in PHWR-Using Thermomechanical Processing for Improving Service Life
61.	Ms. Shrishma Paik	29.08.12	Feasibility of Using Ammonium Di-Uranate Filterate for Stripping of Loaded Solvent in Extraction of Uranium
62.	Shri Rahul Shukla	29.08.12	Development of Resistance Welding Procedure for Welding of Fuel Elements (Zircaloy2) of BWR and its Comparison with Existing Tig Welding
63.	Lt. Cdr. Vikram Singh Jadolia	29.08.12	Design and Development of 27 MHz, 1 KW Solid State RF Power Amplifier
64.	Lt. Col. Manindra Kumar Singh	29.08.12	Digital Implementation and Response Time Optimization of Count Rate Meter to Get Reactor Power and Reactor Period
65.	Shri Santhosh Kumar C. T.	04.09.12	Numerical Simulation of Heat Transfer in a Porous Glass Bed
66.	Shri Uttam Jain	05.09.12	Alumino Thermic Reduction of V2O5-Effects of Slag Chemistry on Vanadium Yield and its Nitrogen Content
67.	Ms. Jothilakshmi	14.09.12	Development of Non-destructive Techniques for Corrosion Monitoring of Austenitic Stainless Steel
68.	Shri Sagar Sonak	14.09.12	Synthesis, Processing and Characterization of Fine Carbide Ceramics
69.	Shri Shantonu Sahoo(BARCTS, Mumbai)VECC	14.09.12	Development of Embedded EPICS for Arm Microcontroller and FPGA Based Soft-Core Processor
70.	Shri Sairam K	15.09.12	Development of B_4C-HfB_2 Composites by Reaction Hot Pressing
71.	Shri Gurpreet Singh Hanspal	18.09.12	Development of Incremental Hinge Technique to Predict the Behaviour of Piping System Subjected to Internal Pressure and Seismic Loading

72.	Shri Abhiram E. R.	18.09.12	Mesh Generation using Stereolithography(STL) Data from Computer Aided Design(CAD) Models
73.	Shri Nikhil Saxena	18.09.12	Study, Implementation and Evaluation of GPU Based Shadow Algorithms and Techniques for Real Time 3D Graphics Application
74.	Ms. Aanchal Srivastava	18.09.12	Mathematical Modeling and Analysis of Current Distribution for Joule Based Ceramic Melter for High Level Waste Vitrification
75.	Shri Sundeep Ghosh(BARCTS, Mumbai)	18.09.12	Stress Analysis of Coil and Associated Structural Components for Superconducting Magnets
76.	Shri Vineet Kumar Dwivedi	01.10.12	Sensitivity Analysis of Resonance Immittance Converter Topologies
77.	Shri Prashant Sharma	17.10.12	Plant Dynamics of PFBR Steam Water System
78.	Shri Pankaj Kumar Kushwaha	18.10.12	Raman Spectroscopy in Presence of Metal Nanostructures
79.	Shri Sudhir Kumar	18.10.12	Quantitative Phase Microscopy of Biological Cells
80.	Ms. Ranjana Rathore	18.10.12	Studies on X-ray Optics
81.	Shri Adya Karthikeyan(NTC, Kudankulam)	18.10.12	Thermal Hydraulic Performance of Nanofluids for a Nuclear Power Plant
82.	Ms. Rinky Dhingra	30.10.12	Electromagnetic Design and Beam Dynamics for a 10 MeV 10 kW Electron Linac
83.	Shri Arihant Kumar Jain(BARCTS, Mumbai)	30.10.12	Improvement in Cathode Test Bench and Measurement of Test Parameters
84.	Shri Sandeep Kumar Singh	30.10.12	Design, Development and Evaluation of a Model Based Master Slave Controller Robust to Communication Delays
85.	Shri M. Vineet	30.10.12	Study and Implementation of Secure Multimedia Communication Protocols
86.	Lt. Cdr. Suguna Kumar	16.11.12	Implementation of Specific Harmonic Elimination Technique in Multi-Level Inverter Through Simulation
87.	Ms. K. Gayathri(NFC)	16.11.12	Design of Algorithm based on Correlation Analysis of Neutronic and Thermal Power Signals for Sensor Fault Detection
88.	Shri Arka Pratap Mitra	16.11.12	Mathematical Modelling and Simulation Studies on Rotating Electric Field Admittance Probe for Void Fraction Measurement

89.	Ms. Sudhakshina Bhattacharya(NTC, Kalpakkam)	16.11.12	Experiments on Formal verification of Some Distributed System Protocols
90.	Ms. Vidhtyalakshmi	16.11.12	Development of Sonar Device for Fuel Subassembly Vibration Measurement
91.	Shri Mahesh Tiwari	16.11 .12	Size Distribution and Chemical Characterization of Combustion Aerosols for Health Hazard Evaluation in Indian Domestic Environments
92.	Ms. Rajeswari Pradhan Rout	16.11.12	A Comparative E Study of Deposition of Radon Decay Products on the Surfaces with their Simulated Deposition in Human Respiratory Tract
93.	Shri Sambamurty Tadde	16.11.12	Studies on the Distribution of Uranium in Ground Water of Tarapur and the Influence of Physico-Chemical Parameters
94.	Shri Shailendra Kumar (NFC)	18.11.12	Performance Evaluation of H_2S Exposed Low Carbon Steel Components of Exchange Towers
95.	Shri Bikram Roy	18.11.12	Design and Development of Photometric based Concentration Measurement System and Ultrasonic based Online Density Measurement System for Uranium Loaded Organic in Solvent Extraction Process
96.	Ms. Urmila Singh	18.11.12	RF Voltage for 1 GeV Proton Accelerator Ring
97.	Shri Mainak Bandyopadhyay	18.11.12	Analytical and Experimental Investigation of Void Fraction in Two Phase Flow System using Ultrasonic Techniques
98.	Shri Manish Kumar Tiwari	18.11.12	Design and Development of EM based Active Liquid Level and Slurry Level Measurement
99.	Shri Mahender Singh	18.11.12	Development of Mechanistic Model for Transient Release of Fission Products for Reactor Fuel under Accident Condition
100.	Shri Kamalkumar Dodiya	18.11.12	Development of Computational Technique for Radiological Data Analysis
101.	Shri Sirisha Gade	18.11.12	Simulsyion Studies of Flue Gas Treatment by Electron Beam
102.	Shri Subrata Patak	18.11.12	Synthesis and Pharmacokinetics study of DOTA peptides labeled with 68Ga & 177Lu and estimation of occupational dose
103.	Shri R. Poorani(NFC)	18.11.12	Development of Modelling Techniques for Dynamic Reliability Analysis
104.	Shri Shib Shankar Sikder	21.11.12	Design of a New Trigger Scheme for MACE Telescope to Detect Pre-Defined Non-Disjoint Events

105.	Shri Kanwarjeet Singh	21.11.12	Evaluation of Tensile Properties and How Behavior of Modified 9Cr-1Mo Steel Clad Tube for Fast Reactors
106.	Shri Ishtiyaq Alam	21.11.12	Prediction of Mean Aactiviy Concentration of Released Radioactive Source using Kalman Filter
107.	Shri Sanjiv Aravamudhan	21.11.12	Modelling and Optimizaion of Desublimer
108.	Shri Nevil Martin Jose	03.12.12	An Investigation on the Transferability of Cohensive Zone Material Parameters for Two Widely used Nuclear Materials
109.	Shri Sai Prasanth(NFC)	11.12.12	Microwave Sintering of Uranium Dioxide Pellets
110.	Shri K. Naga Venkata Sairam	11.12.12	Design of AHWR Steam Drum Level Control System
111.	Shri Sudheer K. Nambiar	11.12.12	Semantic Metadata Harvesting and Archival for Knowledge Domains
112.	Ms. Diana Denice	19.12.12	Life Evaluation of Electronic Modules by Means of Empirical Methods and Accelerated Life Testings
113.	Shri Amit Ahuja	03.01.13	Applying Fault Injection Techniques for Embedded System Reliability Analysis
114.	Shri Prashant Suresh Khubchandani(NTC, Kudankulam)	11.01.13	Reliability Analysis of Passive Heat Removal System of VVER-1000
115.	Shri Trushit Makwana	11.01.13	Reduction of Alpha Activity from Organic Liquid Waste Generated During Fast Reactor Spent Fuel Reprocessing
116.	Shri Pranav Kant Gaur	11.01.13	Developement and accuracy analysis of Coded phase shift 3D scanner
117.	Ms. Usha Pujala	11.01.13	Design of Deuteron RFQ for pulsed Neutron Generator
118.	Ms. Tadimeti Lakshmi Priyanka	11.01.13	Process Modeling & Simulation of Heaters Drains and Vents System of PFBR
119.	Shri Piyush Kumar Aggarwal	11.01.13	CFD Mddeling of Integrated Cold Trap for Primary Sodium Purification in FBR
120.	Shri Sohan lal(BARCTS, Mumbai)	16.01.13	Development of Laser Brazed Joints of AISI 316L SS with Copper
121.	Shri Udbhav Singh Bhadoria	16.01.13	Tribological Evaluation of Rotary CAM Liner of ULVAC PKS-70 Oil Vacuum Rotary Vacuum Pump
122.	Shri Satyasiba Das(NFC)	16.01.13	Process Improvement in 1st Pass Pilgering of Zr-4 PHWR Fuel Tubes by Optimizing Tool Design
123.	Shri Anoop V.	16.01.13	Analysis of Compact Thermal Insulation

124.	Shri Khushboo Singh	16.01.13	Removal of Ruthenium from High Level Liquid Waste (HLLW) Generated During Reprocessing of Spent Fuel
125.	Ms. Vibha Rani Singh(NFC)	16.01.13	Optimisation of phased array ultrasonic probe for nondestructive testing of Zircaloy-4 sheets
126.	Shri Hari Shankar Yadav	23.01.13	Fluidization Process for Agglomeration of Uranium Peroxide Powder
127.	Shri Alok Kumar Gupta	23.01.13	Design and Development of Instrumentation and Control for Positional Drive System of Failed Fuel Location Module of Prototype Fast Breeder Reactor
128.	Shri P. Srijan Babu	23.01.13	Computational Fluid Dynamics Investigations of Lubrication oil Fire in Top Shield Platform of PFBR
129.	Shri Kaushik Ghoshal	02.02.13	Studies on Fabrication, Characterization and Thermo-Physical Property Evaluation of Uranium Rich U-Zr-Nb Ternary Alloy System
130.	Shri Biswajit Sadhu	09.02.13	Structure Determination of Humic Substances Embedded with Radionuclides at Different pH
131.	Shri Avinash Sahu	14.02.13	Catalytic Hydrogenation of Uranyl Nitrate to Uranous Nitrate
132.	Shri Amar Dutt Pant	25.02.13	Standardization of Technique for Characterization and Assessment of Radionuclides Present in Spent Fuel Storage Bay of a Typical Research Reactor
133.	Shri Lokesh Kumar Sharma	03.03.13	Inverse Modelling for Aquatic Source and Transport Parameter Identification
134.	Ms. Archana Soman	05.03.13	Optimization of CaF_2 Particle Size Distribution in Fluoride Neutralization Process and Generation of Parametric Correlation for Scale Up
135.	Shri Tarun Kumar Agarwal	21.03.13	Parameterization and Validation of Computational Fluid Dynamics(CFD) Based Simulating Software to Study the Thoron (^{220}Rn) and its Decay Products Distribution Inside the Confined Environment

Titles of M.Sc.(Engg.) theses for which results were notified during April 1, 2012 to March 31, 2013

Sr.No	Name of the Student	Date of Notification of degree	Thesis Title
1	Shri Mohandas Karamchand Pradhan	03.05.12	Evaluation of Lateral Earth Pressure for Waste Tank Farm due to Static and Seismic Loads and Use of Compressible Geo Fills for its Reduction
2	Shri Pradyumna Kumar Parida	21.11.12	Study of Microstructure and Microchemistry of Dispersoid in Midel ODS Alloy
3	Shri Saju T. Abraham	19.12.12	Assessment of Sensitization in AISI Type 304 Stainless Steel by Non Linear Ultrasonics
4	Shri Y. V. Harinath	21.01.13	Study on Laser Welding of Modified 9Cr-1Mo Steel Clad Tube to End Plug of Metallic Fuel Pins for Fasr Breeder Reactors
5	Shri Manish Kumar	27.02.13	Design, Analysis and Development of Large Size Metallic Mirrors by Vacuum Adaptive Technique

Title of M.Phil thesis for which result was notified during April 1, 2012 to March 31, 2013

Sr.No	Name of the Student	Date of Notification of degree	Thesis Title
1	Shri Ashish Pandey	16.05.12	Determination of Trace Impurities in UO_2, ThO_2 and $(Th, 3.25\%U)O_2$ by Chemical Methods

Annex 7

Receipts & Payments for the financial year

ending on 31.3.2013

The Bombay Public Trusts Act 1950

SCHEDULE VIII

[Vide Rule 17[1]]

Name of the Public Trust:- HOMI BHABHA NATIONAL INSTITUTE, Reg No: F/27776/Mumbai

Deemed University under UGC Act 1956.

BALANCE SHEET AS AT 31-03-2013 (Financial Year 2012-13)

FUNDS & LIABILITIES	AMOUNT (Rs.)	AMOUNT (Rs.)	PROPERTY & ASSETS	AMOUNT (Rs.)	AMOUNT (Rs.)
Trust Funds or Corpus			Immovable Properties		-
Balance as per Last Balance Sheet	-				
Add: Additions during the year	-		Investments		
Other Earmarked Funds			Furniture and Fixtures		
a. Depreciation Fund	-				
b. Sinking Fund	-		Loans (Secured or Unsecured)		
c. Reserve Fund	-		Loans Scholarships	-	
d. Any Other Fund	-		Other Loans	-	
Loans (Secured or Unsecured)			Advances		
a. From Trustees	-		a. To Trustees	-	
b. From Others	-		b. To Employees	-	
			c. To Contractor	-	
Liabilities			d. To Lawyers	-	
a. For Expenses	-		e. To Others	-	
b. For Advances	-				
c. For Rent and Other Deposits	-		Income Outstanding		
d. For Sundry Credit Balances	-		a. Rent	-	
			b. Interest	-	
Income and Expenditure Account			c. Other Income	-	
Balance as per last balance sheet	12,347,731		Cash and Bank Balances		
Less: Appropriation	-		a. Balance in Saving A/c -SBI Bank-HBNI	14,463,682	
Add: Surplus as per Income & Expenditure A/c	2,127,676	14,475,407	b. With the Trustees	-	
			c. With the Manager-Lata B	11,725	14,475,407
Total		14,475,407	Total		14,475,407

Significant Accounting Policies & Notes to Accounts

Income Outstanding -Nil

The above Balance Sheet to the best of our belief contains a true account of the funds and liabilities and of the property and assets of the trust.

As per report of even date

For Vivek V Joshi & Associates

Chartered Accountants

FRN No. 121829W

Vivek V Joshi

Partner

Membership No. 038293

Finance Officer   Dean   Director

शा. आर. बी. ग्रोवर/Dr. R. B. Grover
निदेशक, होमी भाभा राष्ट्रीय संस्थान

Place: Mumbai

Date: 12 AUG 2013

A view of the inner garden of Training School Complex

DIRECTOR
Prof. R. B. Grover
Email : rbrgrover@hbni.ac.in

DEAN
Prof. R. R. Puri
Email : rrpuri@hbni.ac.in
(upto November 30, 2012)

DEAN
Prof. B. K. Dutta
Email : bkdutta@hbni.ac.in
(from December 1, 2012)

ASSOCIATE DEAN AND PUBLIC INFORMATION OFFICER
Dr. R. P. Patel
Email rppatel@hbni.ac.in

For more details, please visit website : www.hbni.ac.in

Back cover page : Training School Complex, Anushaktinagar, Mumbai 400 094