होमी भाभा राष्ट्रीय संस्थान

Homi Bhabha National Institute

शैक्षणिक प्रतिवेदन
Academic Report
2014-2015

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

राष्ट्रीय मूल्यांकन एवं प्रत्यायन परिषद

विश्वविद्यालय अनुदान आयोग का स्वायत्त संस्थान

NATIONAL ASSESSMENT AND ACCREDITATION COUNCIL

An Autonomous Institution of the University Grants Commission

Certificate of Accreditation

The Executive Committee of the
National Assessment and Accreditation Council
on the recommendation of the duly appointed
Peer Team is pleased to declare the
Homi Bhabha National Institute
(Deemed to be University u/s 3 of the UGC Act 1956)
Anushaktinagar, Mumbai, Maharashtra as
Accredited
with CGPA of 3.53 on four point scale
at A grade
valid up to May 10, 2020

Date : May 11, 2015

Director

EC(SC)/07/1.2.1/08

From the Vice-Chancellor

Another year has gone by and I am happy to write for the annual report. During the year, the Council of Management amended Memorandum of Association and Rules to comply with the regulations for deemed to be universities issued by the University Grants Commission. Apart from other changes, the designation of the Principal Executive Officer of the Institute was changed from the Director to the Vice-Chancellor.

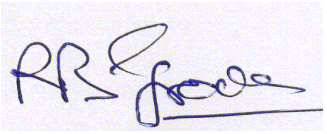
One activity that took a significant part of time of many in the Institute during the first few months of the year was writing the Self-Study Report to be submitted to the National Assessment and Accreditation Council (NAAC). We uploaded the report on the website of the Institute in July 2014. Writing the report was an enriching experience for all of us. A member of the faculty, who was providing inputs for the Constituent Institution he belongs to, said that he learnt several details about his Institute only through the process of providing inputs for the report. As a part of preparation for the review by NAAC, Standing Committee of Deans met several times and documented our practices and this was a very useful exercise in streamlining the working of the Institute. It was the first time that it came to the fore that about 100 individuals associated with the Institute are fellows of prestigious academies and many have won prestigious scientific awards such as Bhatnagar Prize, Homi Bhabha Science & Technology Award, and DAE Lifetime Achievement Award. Overall, the process of preparing for a review by NAAC was stressful, but useful.

NAAC aims to assess and accredit universities and colleges in India. Here one may ask why students come to a university, obviously to acquire education. What is education and what are goals of education? John Locke, in Some Thoughts Concerning Education (1693), named virtue, wisdom, breeding, and learning as goals of education. He seems to stress that creating a scholar is not as important as creating a virtuous man. What is the situation today? I visited web sites of several universities to learn about views on goals of education at the graduate level and came across a variety of views about goals. Educating an individual to be virtuous and ethical continues to be a goal, but continuously expanding stock of information and knowledge, and demands of the

individual self and society have resulted in adding several elements to the list of goals. Here is an attempt to list goals of education: (i) to attain mastery of a broad field of learning, (ii) to engage in and conducting original research, (iii) to effectively communicate knowledge in the discipline, (iv) to demonstrate analytical ability in the discipline, (v) to exhibit best practice, values and ethics of the profession, and (vi) to apply knowledge of the discipline.

One also has to examine an associated question: does education serve the needs of the society or the individual? Certain disciplines can be 'inert' and while an individual may have interest in those topics, society may not benefit from research in such topics. Examples could be aspirations of an individual for erudition or private answers to philosophical questions. Certain disciplines could have immediate application, while certain disciplines may be useful on a long-term basis as they could lead to a better understanding of the universe.

In the case of our Institute, mission of the Department of Atomic Energy (DAE) represents the needs of the society and members of faculty work on topics needing immediate answers as well as those which need to be solved on a longer-term. Funding for research is provided by the Government to work on topics of research as mandated by the mission of the DAE. All students pursuing research in our Institute work on problems that have been identified as related to the mandate of the DAE and in a majority of the cases have immediate application. One can proudly say that in HBNI, we pursue research on relevant topics with a focus on excellence.



(R B Grover)

Introduction

The HBNI has the following as its Constituent Institutions (CIs).

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

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

In 2006, the Government of India decided to strengthen science education and set up institutions for science education and research in various parts of the country. One such institution, the National Institute for Science Education and Research (NISER) was setup at Bhubaneswar by the Department of Atomic Energy (DAE) as a project of the Institute of Physics. Academic programmes of this institute were started as a part of IOP and thereby under HBNI. Steps are being taken to make NISER an independent CI of HBNI.

Academic programmes of the Institute

The HBNI offers a range of academic programmes in chemical sciences, engineering sciences, health sciences, life sciences, mathematical sciences and physical sciences. It also has a programme in strategic studies. Except for NISER, all other institutions conduct programmes at post-graduate level. Various programmes offered are the following.

Ph.D. in varied disciplines is offered at all CIs. HRI and IMSc also offer an integrated Ph.D. programme where students study for **M.Sc.** as well as Ph.D.

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

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

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

Super Specialty Courses at TMC

- **D.M.** (Medical Oncology)
- **M. Ch.** (Surgical Oncology)
- **M. Ch.** (Gynaecological Oncology)

Post Graduate Courses at TMC

- **M.D.** (Pathology)
- **M.D.** (Anaesthesiology)
- **M.D.** (Radio-diagnosis),
- **M.D.** (Radiotherapy),
- **M.D.** (Microbiology), and
- **M.D.** (Immuno Haematology & Blood Transfusion)

DRM: Diploma in Radiation Medicine at BARC.

M.Sc. (Nursing) at TMC.

Dip.R.P.: Diploma in Radiological Physics at BARC.

DMRIT: Diploma in Medical Radio Isotope Techniques at BARC.

The Institute offers a unique Ph.D. programme where students are encouraged to work at the interface of basic research and technology development. Under this programme, they work under the guidance of two supervisors, one having strength in basic research and the other in technology development.

Around 1500 students are pursuing Ph.D. in various disciplines.

All the Constituent Institutions have excellent library facilities having a large collection of books and subscribe to a large number of research journals. All journals are available to researchers on their desktops.

Faculty

Faculty strength in all CIs put together is about 999 CIs, particularly research & development centres have a large number of scientific officers and they provide valuable inputs to research scholars as Technology Advisers. Amongst faculty and scientific officers, there are many who are fellows of prestigious academies, and winners of national and international awards. List of Fellows who are faculty of HBNI are given in the following Tables.

1. Fellows of Indian National Academy of Engineering, New Delhi

S. No.	Name	Year of birth	Year of election	CI
1.	Anil Kakodkar*	1943	1991	BARC
2.	Srikumar Banerjee*	1946	1993	BARC
3.	R.B. Grover*	1949	1999	VC, HBNI
4.	R.K. Sinha	1951	1999	Chairman, CoM
5.	H.S. Kushwaha*	1946	2000	BARC
6.	P. Chellapandi	1956	2001	IGCAR
7.	S.C. Chetal*	1949	2001	IGCAR
8.	T.K. Bera*	1954	2002	BARC
9.	B K Dutta	1953	2004	BARC
10	V.K. Mehra*	1948	2004	BARC
11	Sekhar Basu	1952	2005	BARC
12	T. Jayakumar	1955	2005	IGCAR
13	B.B.Biswas*	1948	2006	BARC
14	S. Venugopal	1955	2006	IGCAR
15	A.K.Bhaduri	1959	2007	IGCAR
16	G K Dey	1957	2008	BARC
17	K. Velusamy	1959	2008	IGCAR
18	R.R.S. Yadav*	1952	2008	BARC
19	U. Kamachi Mudali	1960	2009	IGCAR
20	P.K. Wattal*	1951	2010	BARC
21	K.K. Jayarajan	1962	2011	BARC
22	R. Natarajan	1953	2011	IGCAR
23	K.K. Vaze*	1950	2011	BARC
24	R.K. Singh	1953	2012	BARC
25	A.K. Sinha	1956	2012	BARC
26	S. Chaturvedi	1962	2013	BARC
27	C.K. Pithawa	1951	2013	BARC
28	S.B. Roy	1956	2013	BARC
29	K N Vyas	1957	2014	BARC

2. Fellows of the Indian National Science Academy, New Delhi

	Name	Year of Birth	Year of	CI

			Election	
1.	P.K. Kaw*	1948	1984	IPR
2.	R. Balasubramanian	1951	1988	IMSc
3.	Bikash Sinha*	1945	1989	VECC
4.	Srikumar Banerjee*	1946	1992	BARC
5.	Probir Roy*	1942	1992	SINP
6.	J.B. Joshi*	1949	1995	HBNI
7.	J. Maharana*	1945	1995	IoP
8.	Ashoke Sen	1956	1996	HRI
9.	Romesh Kaul	1952	1998	IMSc
10.	S.K. Apte*	1952	1999	BARC
11.	Swapan K. Ghosh*	1949	1999	BARC
12.	M.K. Sanyal	1954	2001	SINP
13.	A.M. Jayannavar	1956	2002	IoP
14.	B.K. Chakrabarty	1952	2003	SINP
15.	V.S. Sunder	1952	2004	IMSc
16.	Sunanda Banerjee	1952	2005	SINP
17.	Abhijit Sen*	1946	2006	IPR
18.	S.M. Bhattacharjee	1957	2008	IoP
19.	V. Chandrashekar	1958	2008	IOP(NISER)
20.	Y.P. Viyogi*	1948	2009	VECC
21.	R. Gopakumar	1967	2010	HRI
22.	M.V. Hosur*	1950	2010	BARC
23.	Parthasarathi Mitra	1951	2012	SINP
24.	Gautam Bhattacharyya	1966	2013	SINP
25.	S.L. Chaplot	1955	2013	BARC
26.	S. Kailas*	1949	2013	BARC
27.	C.S. Sundar	1952	2013	IGCAR
28.	D. K. Palit	1957	2014	BARC
29.	Anjan Kundu	1953	2014	SINP

3. Fellows of the Indian Academy of Sciences, Bangalore

	Name	Year of Birth	Year of Election	CI
1.	P.K. Kaw*	1948	1974	IPR
2.	R. Balasubramanian,	1951	1987	IMSc
3.	Probir Roy*	1942	1989	SINP
4.	Srikumar Banerjee*	1946	1990	BARC
5.	Swapan K. Ghosh*	1949	1991	BARC
6.	J.B. Joshi*	1949	1991	HBNI
7.	Ashoke Sen	1956	1991	HRI
8.	V.S. Sunder	1052	1992	IMSc
9.	J.K. Bhattacharjee	1952	1993	HRI
10.	Romesh K Kaul	1952	1993	IMSc
11.	J. Maharana*	1945	1994	IoP
12.	S. Kailas*	1949	1995	BARC
13.	Abhijit Sen*	1946	1995	IPR

14.	A.M. Jayannavar	1956	1996	IoP
15.	B.K. Chakraborty	1952	1997	SINP
16.	Anil Kakodkar*	1943	1998	BARC
17.	C.S. Sundar	1952	1999	IGCAR
18.	S.M. Bhattacharjee	1957	2000	IoP
19.	M.K. Sanyal	1954	2001	SINP
20.	Sunanda Banerjee	1952	2002	SINP
21.	V. Chandrashekar	1958	2003	IOP(NISER)
22.	R. Gopakumar	1967	2007	HRI
23.	P.K.Gupta	1954	2007	RRCAT
24.	D.K. Palit	1957	2007	BARC
25.	P. Sankaran	1959	2007	IMSc
26.	S.K. Apte*	1952	2008	BARC
27.	G.K. Dey	1957	2008	BARC
28.	S. Kesavan	1952	2008	IMSc
29.	S.M. Sharma	1952	2008	BARC
30.	D.S. Nagaraj	1958	2010	IMSc
31.	Amita Das	1965	2011	IPR
32.	V. Ravindran	1965	2012	HRI
33.	H.N. Ghosh	1966	2013	BARC
34.	T.K. Nayak	1958	2013	VECC
35.	Arun K. Pati	1966	2013	HRI
36.	A.K. Tyagi	1964	2013	BARC

4. Fellows of the National Academy of Sciences, India, Allahabad

	Name	Year of Birth	Year of Election	CI
1.	P.K. Kaw*	1948	1989	IPR
2.	R. Balasubramanian	1951	1992	IMSc
3.	S.F. D'Souza	1949	1993	BARC
4.	S.K. Apte*	1952	1995	BARC
5.	V.K. Jain	1956	1995	BARC
6.	Abhijit Sen*	1946	1995	IPR
7.	J.K. Bhattacharjee	1952	1997	HRI
8.	S. Kesavan	1952	1997	IMSc
9.	Ashoke Sen	1956	1997	HRI
10.	V.S. Sunder	1952	1997	IMSc
11.	Swapan K. Ghosh*	1949	2001	BARC
12.	Parthasarathi Mitra	1951	2001	SINP
13.	Sumathi Rao	1956	2001	HRI
14.	Probir Roy*	1942	2001	SINP
15.	M.K. Sanyal	1954	2001	SINP
16.	Srikumar Banerjee*	1946	2002	BARC
17.	Anil Kakodkar	1943	2002	BARC
18.	V.C. Sahni*	1945	2002	BARC
19.	K. B. Sainis*	1949	2002	BARC
20.	C.S. Sundar	1952	2002	IGCAR

21.	S. Chattopadhyay	1957	2003	BARC
22.	A.M. Jayannavar	1956	2003	IoP
23.	M. Krishna	1956	2003	IMSc
24.	K. I. Priyadarsini	1959	2003	BARC
25.	P.K. Gupta	1954	2003	RRCAT
26.	P.D.Gupta	1952	2004	RRCAT
27.	H. Pal	1959	2004	BARC
28.	A.K. Tyagi	1964	2004	BARC
29.	S.M. Sharma	1952	2005	BARC
30.	B. Mukhopadhyaya	1966	2006	HRI
31.	D.K. Palit	1957	2006	BARC
32.	P. Sankaran	1959	2006	IMSc
33.	S.D. Adhikari	1957	2007	HRI
34.	S.L. Chaplot	1955	2007	BARC
35.	V.P. Viyogi*	1948	2007	VECC
36.	V. Chandrashekar	1958	2007	IOP(NISER)
37.	H.N. Ghosh	1966	2008	BARC
38.	R.K. Vatsa	1963	2009	BARC
39.	V. Kodiyalam	1966	2010	IMSc
40.	S. Panda	1959	2010	HRI/IoP
41.	A.C. Bhasikuttan	1967	2011	BARC
42.	P.S. Chakraborty	1973	2012	IMSc
43.	D. K. Maity	1964	2012	BARC
44.	D. K. Srivasatava	1952	2012	VECC
45.	Arun K. Pati	1966	2013	HRI
46.	B. Ramakrishnan	1961	2013	HRI
47.	P. D. Naik	1959	2013	BARC
48.	Gautam Bhattacharyya	1966	2013	SINP
49.	T K Ghanty	1963	2014	BARC
50.	J Mohanty (Mrs)	1971	2014	BARC

5. *Fellow of National Academy of Agricultural Sciences*

	Name	Year of Birth	Year of Election	CI
1.	S K Apte*	1952	1998	BARC

6. *Fellows of the Third World Academy of Sciences, Trieste, Italy*

	Name	Year of Birth	Year of Election	CI
1.	Ashoke Sen	1956	2004	HRI
2.	Srikumar Banerjee*	1946	2007	BARC
3.	G. Baskaran*	1948	2008	IMSc
4.	J.B. Joshi*	1949	2008	HBNI
5.	V. Chandrashekar	1958	2008	IoP(NISER)
6.	Swapan K. Ghosh*	1949	2010	BARC

7. *Fellow of World Academy of Art and Science*

	Name	Year of Birth	Year of Election	CI
1.	R.B. Grover*	1949	2013	VC HBNI

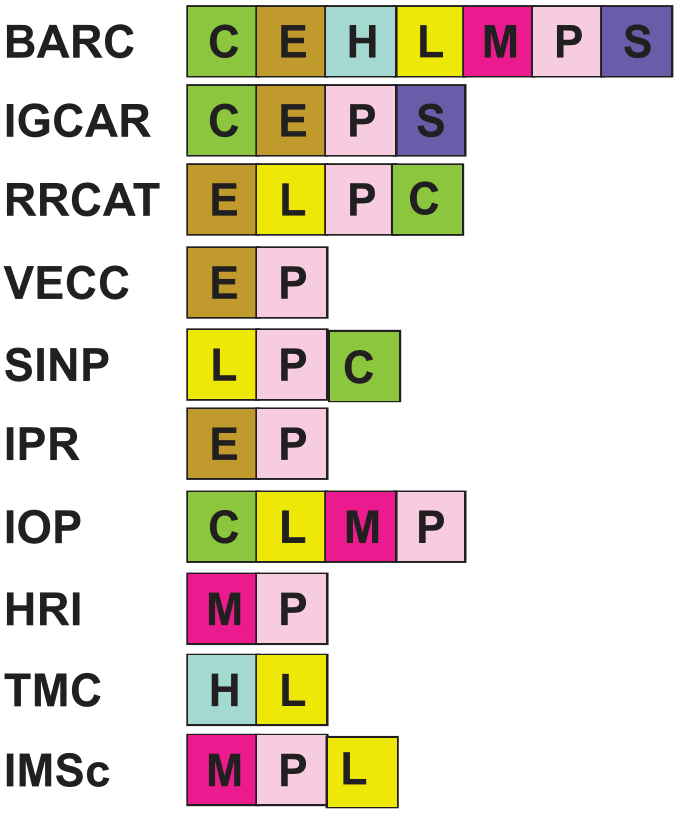
Annex 1

Composition of the Bodies of the Institute

Management of the Institute

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

- Chemical Sciences (C)
- Engineering Sciences (E)
- Health Sciences (H)
- Life Sciences (L)
- Mathematical Sciences (M)
- Physical Sciences (P)
- Strategic Studies (S)



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

Advisory Committee

Dr. R. K. Sinha, Chairman, AEC	Chairman
Prof. R. B. Grover Director, HBNI	Member
Dr. S. Basu Director, BARC	Member
Prof. P. R. Vasudeva Rao Director, IGCAR	Member
Prof. P.D.Gupta Director, RRCAT	Member
Prof. Dinesh Srivastava Director, VECC	Member
Prof. D. Bora Director, IPR	Member
Prof. B. K. Chakrabarti Director, SINP	Member
Prof. R. A. Badwe Director, TMC	Member
Prof. R. Balasubramanian Director, IMSc	Member
Prof. Sandip Trivedi Director, TIFR	Member
Prof. V. Chandrashekar Director, NISER	Member
Prof. J. K. Bhattacharjee Director, HRI	Member
Prof. Ajit Srivastava / Sudhakar Panda Director, IoP	Member
Prof. 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. G.Amarendra
   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. Ramesh Anishetty
   Institute of Mathematical Sciences
9. Prof. S.K.Gupta
   Bhabha Atomic Research Centre
10. Prof. S L Chaplot
    Bhabha Atomic Research Centre

Chemical Sciences

1. Prof. B.N.Jagtap **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. B.S.Tomar
   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
10. Prof. D. K. Palit
    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 Rajiv Sarin
   Advanced Centre for Treatment,
   Research & Education in Cancer
   (ACTREC)
4. Prof H.S.Mishra
   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
   Saha Institute of Nuclear Physics

Engineering Sciences

1. Prof. P.K. Vijayan **Convener**
   Bhabha Atomic Research Centre
2. Prof. G. K. Dey
   Bhabha Atomic Research Centre
3. Prof. R. C. 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. K.Velusamy
   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

Permanent Invitee

1. Prof. S.Mukherjee
   Institute of Plasma Research

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. R.R.Puri
   IIT Gandhinagar
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
10. Prof. Adimurthi
    TIFR, Bangalore

Strategic Studies

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

2. Dr. K.Raghuraman
   Ex-DAE, Navi Mumbai
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

Health Sciences

1. Prof. K. S. Sharma **Convener**
   Tata Memorial Centre, Mumbai
2. Prof. D. D. Deshpande
   Tata Memorial Hospital, Mumbai
3. Dr. N.Roy
   Bhabha Atomic Research Centre, Mumbai
4. Prof. S. K. Srivastava
   Tata Memorial Hospital, Mumbai
5. Dr. P.S. Yadav
   Tata Memorial Hospital, Mumbai
6. Dr. S. B. Banavali
   Tata Memorial Hospital, Mumbai
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

Undergraduate Studies

1. Prof. V.Chandrashekhar -**Convener**
   NISER, Bhubhaneshwar.
2. Prof. V.Muruganandam
   NISER, Bhubhaneshwar
3. Prof. Pinaki Mazumdar
   HRI, Allahabad
4. Prof. V.K.Jain
   BARC, Mumbai
5. Prof. Amritanshu Prasad
   IMSc, Chennai
6. Prof. S.K.Apte
   BARC, Mumbai

Officers of the Institute

Academic

Prof. R.B. Grover	Director
Prof. B.K. Dutta	Dean
Prof. D. K. Maity	Associate Dean
Dr. A.K. Dureja	Associate Dean (w.e.f. 01.12.2014)

Administrative and Accounts

Shri Himanshu Shankar	Finance Officer
Ms. B. Lata	Administrative Officer

Deans-Academic at the CIs

BARC

Prof. S.K. Apte	Life Sciences (Coordinating Dean at BARC for HBNI)
Prof. G.K. Dey	Engineering Sciences
Prof. A. K. Mohanty	Physical Sciences
Prof. B. S. Tomar	Chemical Sciences
Prof. Sandip Basu	Health 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 Sciences

HRI

Prof. Pinaki Majumdar

IMSc

Prof. Vijay Kodiyalam	Mathematical Sciences
Prof. Ghanashyam Date	Physical Sciences
Prof. Gautam Menon	Life Sciences

IoP

Prof. Ajit Srivastava

IoP-NISER

Prof. V. Muruganandam

IPR

Prof. S. Mukherjee

SINP

Prof. P. Mitra

TMC

Prof. K. S. Sharma

Annex 2

Standing Committees

Standing Academic Committees

BARC

Physical Sciences & Mathematical Sciences

1.	Dr. S.L. Chaplot	Chairman
2.	Dr. S. M. Sharma	Member
3.	Dr. V. M. Datar	Member
4.	Dr. Satish Gupta	Member
5.	Dr. K. C. Mittal	Member
6.	Dr. P. D. Krishnani	Member
7.	Dr. N. K. Sahoo	Member
8.	Dr. D.N. Sharma	Member
9.	Dr. Amar Sinha	Member
10.	Dr. Vinod Kumar	Member
11.	Dr. B. N. Jagatap	Convener

Chemical Sciences

1.	Dr. K.L. Ramakumar	Chairman
2.	Dr. B. N. Jagatap	Member
3.	Dr. S.K. Aggarwal	Member
4.	Dr. A. K. Goswami	Member
5.	Dr. D. K. Palit	Member
6.	Dr. A V R Reddy	Member
7.	Dr. S. Chattopadhyay	Member
8.	Dr. B. S. Tomar	Member
9.	Dr. L. Vashney	Member
10.	Dr. S. Velumurugan	Member
11.	Dr. (Smt.) Sharmila Banerjee	Member
12.	Dr. V. K. Jain	Convener

Life Sciences

1.	Dr. S. K. Apte	Chairman
2.	Dr. A. K. Sharma	Member
3.	Dr. M. G. R. Rajan	Member
4.	Dr. J. R. Bandekar	Member
5.	Dr. S. P. Kale	Member
6.	Dr. N. Jawali	Member
7.	Dr. (Smt.) Hema Rajaram	Convener

Engineering Sciences & Strategic Studies

1.	Dr. S. Banerjee	Chairman
2.	Dr. L. M. Gantayet	Member
3.	Dr. P. K. Tiwari	Member
4.	Dr. R. K. Singh	Member
5.	Dr. P. K. Vijayan	Member
6.	Dr. G. K. Dey	Member
7.	Dr. V. K. Suri	Member
8.	Dr. P. V. Varde	Member
9.	Dr. D. N. Badodkar	Member
10.	Dr. Kallol Roy	Member
11.	Dr. A. P. Tiwari	Convener

Health Sciences

1.	Dr. M. G. R. Rajan	Chairman
2.	Dr. Pradeepkumar K. S.	Member
3.	Dr. R. M. Tripathy	Member
4.	Dr. (Smt.) S. Banerjee	Member
5.	Dr. B. K. Sapra	Member
6.	Dr. M. S. Kulkarni	Member
7.	Dr. Biriajalaxmi Das	Member
8.	Dr. S. D. Sharma	Member
9.	Dr. Gaurav Malhorta	Member
10.	Dr. Sandip Basu	Convener (DRM, DMRIT, MPhil,PhD)
11.	Shri Appala Raju Babu	Convener (DipRP)

IGCAR

Physical Sciences

1.	Dr. G. Amarendra	Chairman
2.	Dr. M.Vijialakshmi	Member
3.	Dr. B.Venkatraman	Member
4.	Dr. M. Sai Baba	Member
5.	Dr. B. K. Panigrahi	Member
6.	Dr. A. Bharathi	Member
7.	Dr. K. Devan	Member
8.	Dr. A.K. Tyagi	Member
9.	Dr. John Philip	Member
10.	Dr. M. T. Jose	Member
11.	Dr. Sandip Kumar Dhara	Member
12.	Dr. N. Subramanian	Member
13.	Dr. B.V.R. Tata	Convener

Chemical Sciences

1.	Dr. K. Nagarajan	Chairman
2.	Dr. V. Ganesan	Member
3.	Dr. U. Kamachi Mudali	Member
4.	Dr. A. Bharathi	Member

5.	Dr. N. Sivaraman	Member
6.	Dr. C. Mallika	Member
7.	Dr. V. Jayaraman	Member
8.	Dr. M. Sai Baba	Member
9.	Dr. K. V. G. Kutty	Member
10.	Dr. S. Anthonysamy	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. K. Velusami	Member
7.	Dr. B.P.C. Rao	Member
8.	Dr. Saroja Sai Baba	Member
9.	Dr. K.Nagarajan	Member
10.	Dr. M. Sai Baba	Member
11.	Dr. G. Sasikala	Convener

VECC

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

RRCAT

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.M.Oak	Member
8.	Shri P. R.Hannurkar	Member
9.	Dr. Arup Banerjee	Member
10.	Dr. A. Chowdhury	Member
11.	Dr. S. B. Roy	Convener

IPR

1.	Dr S Mukherjee	Chairman
2.	Dr 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

HRI

Physical Sciences

1.	Dr. Dileep Jatkar	Convener
2.	Dr. Pinaki Majumdar	Member
3.	Dr. Anshuman Maharana	Member
4.	Dr. Anirban Basu	Member
5.	Dr. T. P. Pareek	Member

Mathematical Sciences

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2.	Dr. Rukmini Dey	Member
3.	Dr. S D Adhikari	Member

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1.	Dr. A. M. Jayanavar	Chairman
2.	Dr. S. K. Patra	Member
3.	Dr. D. Topwal	Member
4.	Dr. S. K. Agarwalla	Member
5.	Dr. G. Tripathy	Convener

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3.	Dr. V. Muruganandam	Member
4.	Dr. A. Srinivasan	Member
5.	Dr. V. Krishna Kumar	Member
6.	Dr. Palok Aich	Member
7.	Dr. Vidyanand Nanjundiah, IISc	Member
8.	Dr. Sandeep Vaerma, IIT Kanpur	Member
9.	Dr. V. Ravishankar,	Member

	IIT Delhi	
10.	Dr. Srinivas Vasudevan, TIFR	Member
11.	Dr. Praful Singru	Member
12.	Dr. Moloy Sarkar	Member
13.	Dr. Anil Kumar Karn	Member
14.	Dr. Bedangadas Mohanty	Member
15.	Dr. Pranay K. Swain	Member
16.	Dr. Harapriya Mohapatra	Member
17.	Dr. D. K. Maity, HBNI	Member
18.	Dr. A. K. Naik	Convener

IMSc Standing Committee

Computational Biology

1.	Dr. Gautam I Menon	Convener
2.	Dr. Sitabhra Sinha	Member
3.	Dr. Rahul Siddharthan	Member
4.	Dr. Areejit Samal	Member
5.	Dr. Satyavani Vemparala	Member

Mathematics

1.	Dr. Partha Sarathi Chakraborty	Convener
2.	Dr. Parameswaran Sankaran	Member
3.	Dr. V. S. Sunder	Member
4.	Dr. S. Viswanath	Member

Theoretical Computer Science

1.	Dr. Kamal Lodaya	Convener
2.	Dr. V. Arvind	Member
3.	Dr. C.R. Subramanian	Member
4.	Dr. Meena Mahajan	Member
5.	Dr. Saket Saurabh	Member
6.	Dr. Sayan Bhattacharya	Member
7.	Dr. Venkatesh Raman	Member
8.	Dr. Vikram Sharma	Member

Physics

1.	Dr. V S Nemani	Convener
2.	Dr. D. Indumati	Member
3.	Dr. Sanatan Digal	Member
4.	Dr. Sujay R. Ashok	Member
5.	Dr. R. Shankar	Member
6.	Dr. R. Rajesh	Member
7.	Dr. Ganesh Ramachandran	Member
8.	Dr. Srihari Gopalakrishna	Member
9.	Dr. Kalyana Rama	Member
10.	Dr. Ronojoy Adhikari	Member

TMC Standing Committee

Life Sciences

1.	Dr. S V Chiplunkar	Convener
2.	Dr. N.V. Shirsat	Member
3.	Dr. R. Kalraiya	Member
4.	Dr. S N Dalal	Member
5.	Dr. Tanuja Teni	Member

Health Sciences

1.	Dr. D.A. Chaukar	Convener
2.	Dr. K. George	Member
3.	Dr. N.C. Purandare	Member
4.	Dr. Prachi Patil	Member
5.	Dr. Madhavi Shetmahajan	Member
6.	Dr. V.M. Noronha	Member
7.	Dr. Munita Bal	Member

Annex 3

Faculty List (April 1, 2014 to March 31, 2015)

BARC

Chemical Sciences

1. Achary S.N.
2. Acharya R.
3. Achuthan P.V.
4. Agarwal Renu (Ms.)
5. Aggarwal S.K.
6. Ali SK. Musharaf
7. Arya Ashok Kumar
8. Bandyopadhyay Tusar
9. Banerjee A. (Ms.)
10. Banerjee Sharmila (Ms.)
11. Bharadwa. S.R. (Ms.)
12. Bhardwaj Y.K.
13. Bhasikuttan A.C.
14. Bindal R.C.
15. Chakraborty Sudipta (Ms.)
16. Chandrakumar K.R.S.
17. Chattopadhyay Subrata
18. Chaudhury Niharendu
19. Choudhury Sharmistha Dutta (Ms.)
20. Chowdhury D.P.
21. D. Alamelu (Ms.)
22. Das D. (RRF)
23. Das Tapas
24. Das Tomi Nath
25. Dash Smruti (Ms.)
26. Dash Ashutosh
27. Dey Ghasiram
28. Dey Sandip
29. Dhanya S.
30. Dutt G.B.
31. Dutta Dimple (Ms.)
32. Ganguly R.
33. Ghanty Tapan Kumar
34. Ghosh Asim Kumar
35. Ghosh Hirendra Nath
36. Ghosh Subir Kumar
37. Ghosh Sunil K.
38. Ghosh Swapan K. (RRF)
39. Goswami Madhumita (Ms.)
40. Goswami A.
41. Grover Vinita (Ms.)
42. Hassan P.A.
43. Jain V.K.
44. Jha S.K.
45. Kadam R.M.
46. Kannan S.
47. Kapoor Sudhir
48. Kaushik C.P.
49. Kedarnath G.
50. Korde Aruna (Ms.)
51. Kshirsagar R.J.
52. Kumar Abhinav Dubey
53. Kumar Awadhesh
54. Kumar Manmohan
55. Kumar Sangita D. (Ms.)
56. Kumar Virendra
57. Kumar Sanjukta A. (Ms.)
58. Maity Dilip K.
59. Majumder C.
60. Meera Venkatesh (Ms.)
61. Mishra N.L.
62. Mishra R.
63. Mohanty Jyoti (Ms.)
64. Mohapatra Prasanta Kumar
65. Mukherjee S.K.
66. Murali M.S.
67. Naik Devidas B.
68. Naik Prakash D.
69. Naik Y. P.
70. Natarajan V.
71. Nath Sukhendu
72. Nayak A.K.
73. Nayak Sandip Kumar
74. Ningthoujam Raghumani Singh
75. Pabby Anil Kumar
76. Padmanabhan P.V.A.
77. Pai Mrinal (Ms.)
78. Pal Haridas
79. Palit Dipak K.
80. Pandey A.K.
81. Pandey Usha
82. Pandit Gauri G. (Ms.)
83. Parida S.C.
84. Patra Chandra Nath
85. Pradeep Kumar
86. Pujari Pradeep Kumar
87. Raje Naina (Ms.)
88. Ramakumar K.L.
89. Ramamoorthy N.
90. Ramkumar Jayashree (Ms.)
91. Rangarajan S.
92. Rath M. S.
93. Ravi P.M.
94. Ray A.K.
95. Reddy A.V. R.
96. Roy Mainak
97. Sali S.K.
98. Samanta Alok K
99. Sanjiv Kumar
100. Sasikala R. (Ms.)
101. Satpati Ashish Kumar
102. Sawant Shilpa N. (Ms.)
103. Sharma Anubha
104. Sharma Pramod
105. Shrivastav Ritu M. (Ms.)
106. Singh Ajay K.

107. Singh Dhruva Kumar
108. Singhal Anshu (Ms.)
109. Singhal Rakesh Kumar
110. Sodaye Hemant S.
111. Sodaye Suparna (Ms.)
112. Sreenivas T.
113. Srinivasan M.P.
114. Sudarshan Kathi
115. Sudarsan V.
116. Sunil Jai Kumar
117. Sunil Sabharwal
118. Sunny Fabby (Ms.)
119. Tomar B.S.
120. Tripathi A.K.
121. Tripathi R.M.
122. Tripathi S.C.
123. Tyagi A.K.
124. Upadhyaya Hari Prasad
125. Varshney Lalit
126. Vatsa R.K.
127. Velmurugan S.
128. Verma Rakesh

Engineering Sciences

1. Awasthi Alok
2. Badodkar D.N.
3. Balasubramaniam R.
4. Banerjee S.
5. Betty C. A. (Ms.)
6. Bhargava Kapilesh
7. Bhattacharjee Anup K.
8. Bidaye A. C.
9. Chakraborty S.P.
10. Chakravartty J.K.
11. Chakravarty Anindya
12. Chattopadhyay J.
13. Chaturvedi Shashank
14. Das Ramakrishna
15. Dey G.K.
16. Dutta B.K.
17. Dwarakanath T.A.
18. Ghosh A. K. (RRF)
19. Gopalakrishnan Sugilal
20. Grover R.B.
21. Kain Vivekanand
22. Kapoor Rajeev
23. Kar D.C.
24. Khan K.B.
25. Mahata Tarasankar
26. Maheshwari N.K.
27. Mukhopadhyay Sulekha (Ms.)
28. Nayak Arun Kumar
29. Pal Sangita (Ms.)
30. Pal Prabir Kumar
31. Patankar V.H.
32. Prakash Deep
33. Ravindranath S.V.G.
34. Reddy G.R.
35. Roy Debanik
36. Roy Kallol
37. Roy S. B. (Ms.)
38. Samal M.K.
39. Sarvana Kumar U
40. Satya Sai P.M.
41. Sengupta Pranesh
42. Sharma Archana (Ms.)
43. Singh J.B.
44. Singh R.K.
45. Singh R.N.
46. Srivastava D.
47. Suri A. K. (RRF)
48. Taliyan S.S.
49. Tewari P.K. (RRF)
50. Tewari R.
51. Tiwari A.P.
52. Topkar Anita V. (Ms.)
53. Tripathy P. K.
54. Varde Prabhakar V.
55. Vijayan P.K.
56. Vincent Tessy (Ms.)
57. Vinod Gopika (Ms.)
58. Vinod Kumar A.

Health Sciences

1. Basu Sandip
2. Malpani B.L.
3. Sharma Sunil Dutt
4. Gaurav Malhotra

Life Sciences

1. Acharya Celin
2. Apte S.K.
3. Badigannavar Anand M.
4. Ballal Anand D.
5. Bhilwade H.N.
6. Chawla S. P.
7. Chitela Rajanikant
8. Das Birajalaxmi (Ms.)
9. Fulzele Devanand Pralhadrao
10. Ganapathi T.R.
11. Gautam Satyendra
12. Ghosh Anu
13. Gopalakrishnan Roja (Ms.)
14. Jambhulkar Sanjay
15. Jamdar S.N.
16. Kale Sharad P.
17. Kulkarni Savita (Ms.)

18. Kulkarni V.M.
19. Kumar Mukesh
20. Kumar S. Santosh
21. Kumar Vinay
22. Manjaya J. G.
23. Maurya Dharmendra Kumar
24. Melo J.S.
25. Misra Hari S.
26. Mukherjee Archana (Ms.)
27. Mukherjee Prasun Kumar
28. Mukhopadhyaya Rita (Ms.)
29. Nancharaiah Y.V.
30. Pandey B.N
31. Patro Birija Sankar
32. Priyadarsini Indira (Ms.)
33. Rajan M.G.R.
34. Rajaram Hema (Ms.)
35. Rao Toleti Subba
36. Reddy Kandali S.
37. Saini Ajay
38. Shankar Bhavani S.
39. Rath Devashish
40. R. Shashidhar
41. Souframanien
42. Subramanian Mahesh
43. Chatterjee Suchandra (Ms.)
44. Suprasanna P.
45. Uppal Sheetal (Ms.)
46. Variyar Prasad
47. Venugopalan V.P.

Physical Sciences

1. Ahmed Zafar
2. Aswal D.K.
3. Aswal V.K.
4. Bakshi Ashok Kumar
5. Bandyopadhyay Tapas
6. Basu Saibal
7. Bera S.
8. Bhattacharyya Dibyendu
9. Biswas Debabrata
10. Biswas Dhruba J.
11. Biswas Dipak Chandra
12. Chaplot S.L.
13. Chaturvedi Shashank
14. Chauhan A. K.
15. Das Amitabh
16. Dasgupta K.
17. Datar V.M.
18. Datta Debabrata
19. Debnath A.K.
20. Degwekar S.B.
21. Deo Mukul Narayan
22. Dev Vas
23. Divakar Rao K.
24. Dutta Dipanwita (Ms.)
25. Gadkari Sanjay C.
26. Gaitonde D.M.
27. Ghorui Srikumar
28. Goswami B.K.
29. Gupta Anurag
30. Gupta N.K.
31. Gupta S.C.
32. Gupta Shiv Kumar
33. Jagatap B.N.
34. Jain Sudhir Ranjan
35. Jha S. N.
36. John Bency V.
37. Kannan Umasankari (Ms.)
38. Karmakar Debjani (Ms.)
39. Kaushik T.C.
40. Koul Dileep Kumar
41. Krishnani P.D.
42. Kulkarni Mukund S.
43. Kumar Aniruddha
44. Kumar Mukesh
45. Kumar Vinay
46. Kshirsagar Mukul Narayan
47. Mahata Kripamay
48. Manohar K.G.
49. Mazumder Subasish
50. Mishra Adya Prasad
51. Mishra D.R.
52. Mishra Rosaline
53. Mitra A.K.
54. Mitra S.
55. Mittal Ranjan
56. Mohan Pant Lalit
57. Mohanty Ajit Kumar
58. Mukhopadhyay Ramaprasad
59. Murali Chitra (Ms.)
60. Nakhate S.G.
61. Nayak B.K.
62. Nilaya J. Padma (Ms.)
63. Pradhan S.
64. Rajarajan A.K.
65. Ramaniah Lavanya M. (Ms.)
66. Rannot R.C.
67. Rao P.M. (Ms.)
68. Rao Mala (Ms.)
69. Rao Turumella V. Chandrasekhar
70. Ravikumar G.
71. Ray Aditi (Ms.)
72. Roy Bidyut Jyoti
73. Sahoo N.K.
74. Sahu S. K.
75. Sakuntala T.
76. Salunke H. G.

77. Sangeeta Ms.
78. Santra Satyaranjan
79. Sapra B.K. (Ms.)
80. Sastry P. Umamaheswara
81. Saxena Alok
82. Sekhar B.N. Raja
83. Selvam T. Palani
84. Sen Debasis
85. Sharma Surinder M.
86. Shastri Aparna (Ms.)
87. Shrivastava Aradhana
88. Shukla Prashant
89. Singh Ajay
90. Singh Pitamber
91. Sinha Amar
92. Sinha Sucharita (Ms.)
93. Suryanarayana M.V.
94. Tickoo A.K.
95. Udupa D. V.
96. Warrier Manoj Kumar
97. Yusuf S.M.

Strategic Studies

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

HRI

Physical Sciences

1. Basu Anirban
2. Bhattacharjee J.K.
3. Choubey Sandhya (Ms.)
4. Das Tapas Kumar
5. Datta Asesh Krishna
6. De Aditi Sen (Ms.)
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. Pareek T.P.
16. Pati Arun Kumar
17. Rai Santosh K.
18. Rao Sumathi (Ms.)
19. Ravindran V.
20. Sen Ashoke
21. Sen Prasenjit
22. Sen Ujjwal

Mathematical Sciences

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

IGCAR

Chemical Sciences

1. Ananthasivan K.
2. Anthonysamy S.
3. Antony M.P.
4. Das Arindam
5. Ganesan Rajesh
6. Gnanasekar K.I.
7. Jayaraman V.
8. Jena Hrudananda
9. Joseph M.
10. Mallika C. (Ms.)
11. Mudali U. Kamachi
12. Narasimhan T.S. Lakshmi
13. Panigrahi Bhabani Shankar
14. Prabhakara Reddy B.
15. Ponraju D.
16. Pujar M.G.
17. Rao P.R. Vasudeva
18. Sai Baba M.
19. Satpathy K.K.
20. Sivaraman N.
21. Sundararajan K.

Engineering Sciences

1. Albert Shaju K.
2. Basu Joysurya
3. Bhaduri Arun K.
4. Chellapandi P.
5. Choudhary B. K.
6. Jayakumar T.
7. Kumar Anish
8. Laha Kinkar
9. Mathew M.D.
10. Moitra Aniruddha

11. Mudali U. Kamachi
12. Mukhopadhyay C.K.
13. Murugan S.
14. Parmeswaran P.
15. Ramachandran Divakar
16. Rao B. Purna Chandra
17. Saibaba Saroja (Ms.)
18. Sasikala G. (Ms.)
19. Sharma Anil Kumar
20. Srinivasan V.S.
21. Valsan M.
22. Vasudevan M.
23. Velusamy K.
24. Venugopal S.

Physical Sciences

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

`IMSc

Mathematical Sciences

1. Arvind V.
2. Balasubramanian R.
3. Chakraborty Partha Sarathi
4. Chatterjee Pralay
5. Gun Sanoli (Ms.)
6. Iyer Jaya N. (Ms.)
7. Kesavan S.
8. Kodiyalam
9. Krishna M.
10. Lodaya Kamal
11. Mahajan Meena (Ms.)
12. Mohari Anilesh
13. Mukhopadhyay Anirban
14. Nagaraj D.S.
15. Prasad Amritanshu
16. Raghavan K.N.
17. Raman V.
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23. Sinha Rahul
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Physical Sciences

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5. Parui Sanjay
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8. Gowdigere Chetan N.
9. Mal Prolay Kumar
10. Mohanty Bedangadas
11. Mohapatra Ashok
12. Sahoo Pratap Kumar
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Physical Sciences

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6. Basu Chinmay
7. Basu Padmanava
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9. Bhattacharya Satyaki
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38. Venkatraman Prasanna
39. Venugopalareddy B. V.
40. Waghmare Sanjeev K.

Physical Sciences

1. Deshpande D.D

Annex 4

Abstracts of Ph.D. Theses

(April 1, 2014 to March 31, 2015)

Name	:	**Vijay Kumar Sohani**
Enrolment No.	:	MATH08200704002
Date of Award of degree	:	21.04.14
Constituent Institute	:	Harish-Chandra Research Institute
Title	:	Nonlinear Schrodinger Equation and the Twisted Laplacian

Abstract

During my Ph.D., I studied well posedness results for nonlinear Schrodinger equation for the twisted Laplacian and also for the Laguerre operator. A brief description of the work is given below.

Nonlinear Schrodinger equation for the twisted Laplacian:
We consider the initial value problem for the nonlinear Schrodinger equation associated to the twisted Laplacian for a general class of nonlinearity which includes the power type nonlinearity. We consider first order Sobolev space defined in terms of first order differential operators which commute with Schrodinger propagator for the twisted Laplacian. In this Sobolev space we establish the local well posedness of the initial value problem for the nonlinear Schrodinger equation on C^n. Our approach is based on Strichartz type estimates and fixed point argument. This work is appeared in J. Funct. Anal. 265 (1) (2013) 1-27. This is a joint work with Prof. P. K. Ratnakumar.

Nonlinear Schrodinger equation and the twisted Laplacian- Global well posedness:
The Sobolev space considered above is not the energy space, therefore one can not conclude energy conservation. We overcome this situation by introducing the energy Sobolev space defined using the certain first order differential operators. Though these operators do not commute with the Schrodinger propagator for the twisted Laplacian, they have a quasi commutative relation, suitable for us. The advantage of working with this Sobolev space is that we get energy conservation in this case. The global well posedness is then deduced via a blowup analysis, with the help of the mass and the energy conservation established here. This is a joint work with Prof. P. K. Ratnakumar.

Nonlinear Schrodinger equation for the twisted Laplacian in the critical case :
The method for proving existence of solutions in subcritical cases discussed above will not work in the critical case, as we do not have suitable Strichartz estimates. We overcome this situation by using the truncation argument of Cazenave and Weissler (Nonlinear Semigroups, Partial Differential Equations and Attractors, Lect. Notes Math. 1394, Springer 1989, 18-29) and reduce the problem to the subcritical case for which we can prove the existence of solution. We obtain solution to the original problem by limiting argument and by using the Strichartz estimates.
Strichartz estimates for the Schrodinger propagator for the Laguerre operator :

In this work (Proc. Indian Acad. Sci. (Math. Sci.), 2013, 123 (4), 525-537), we consider the n-dimensional Laguerre operator and establish the Strichartz estimates for the Schrodinger propagator for the Laguerre operator. Using these estimates, we prove the local well posedness of the initial value problem for the Schrodinger equation in the L^2 space associated to the Laguerre operator.

Publications

1. (with P. K. Ratnakumar) Nonlinear Schrodinger equation for the twisted Laplacian, J. Funct. Anal., 2013, 265 (1), 1-27.
2. Strichartz estimates for the Schrodinger propagator for the Laguerre operator, Proc. Indian Acad. Sci. (Math. Sci.), 2013, 123 (4), 525-537.
3. (with P. K. Ratnakumar) Nonlinear Schrodinger equation for the twisted Laplacian- global well posedness, communicated.
4. Nonlinear Schrodinger equation for the twisted Laplacian in the critical case, communicated.

Name	:	**Satyabrata Mishra**
Date of Award of degree	:	21.04.14
Enrolment No.	:	CHEM02200704008
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	Studies on Development of Process Related Issues in Aqueous Reprocessing of Fast Reactor Spent Fuels

Abstract

The high level liquid waste (HLLW) resulting from the solvent extraction step in the reprocessing of spent fuels of Fast Breeder Reactors (FBRs) contains fission and corrosion products in about 4 M nitric acid. Removal of nitric acid from the HLLW is warranted for the reduction of volume, minimization of corrosion in waste tanks during subsequent storage of concentrated waste solution as well as to simplify the procedure for waste fixing. During the extraction stage, owing to high dose of radiation, the solvent and the diluent employed in the extraction process undergo chemical, thermal and radiolytic degradation resulting in a number of degraded products with varying physiochemical properties. Accumulation of the degradation products in the solvent can lead to damages like increase in loss of U and Pu in the raffinate, formation of emulsions and cruds at the liquid-liquid interface which disturb the continuous extraction process and the evolution of physiochemical properties of the phases, mainly viscosity and interfacial tension. Also during extraction, due to the mutual solubility of solvent TBP in FTNCL, the HLLW contains a small amount of TBP, which undergoes hydrolysis to non-volatile species. When liquid waste is concentrated at high temperatures in evaporators, exothermic reactions occur due to the decomposition of TBP-associated compounds. Removal of dissolved TBP is thus, desirable for the safe operation of the plant.

In the present thesis, electrochemical reduction of 4 M nitric acid was carried out under constant potential and current conditions. The rate constant was computed from the batch mode experimental data using kinetic equations. The performance of anodes of different surface area (SA) was compared in the reduction process. The temperature of the cell was significantly reduced when anode of higher SA was used. Failure of Pt electroplated Ti anodes after 450 h implies that plated anodes should be used only at low current density in order to extend their life. Reaction bonded silicon nitride tube fabricated indigenously performed better than the imported commercial tube as diaphragm in electrolytic cells.

Continuous and safe denitration was demonstrated in full-scale plant capacity using pure nitric acid and synthetic waste solutions using formaldehyde as reductant. At temperatures above 98°C the induction period was 1 - 2 min. The reaction efficiency was computed to be in the range 70-80 %. Destruction was successfully carried out without antifoaming agents though severe foaming could be observed in the synthetic solutions with metallic fission products. Volume reduction of 10 % could be achieved in the overall denitration reaction.

Thermal as well as radiolytic degradation behavior of TBP diluted with Dodecane/NPH in the presence/absence of nitric acid was investigated. Thermal degradation at 40°C for 800 h or at 60°C for 400 h did not alter significantly the physiochemical properties, but metal retention was observed to be significant. Radiolysis up to 20 MRad brought marginal change in density, viscosity and PDT. Beyond 10 MRad, significant amount of Zr gets retained by organic phases. Irradiation to a higher dose of 100 MRad indicated the formation of new classes of compounds. TBP-DD system exhibited better stability than the TBP-NPH system.

The solubility of TBP in nitric acid (0 - 14 M) was measured in the range 25 to 60°C. With increase in temperature solubility increased. Fission products (Zr and Ru) increased the solubility of TBP in aqueous phase whereas uranium decreased its solubility. The solubility data were correlated to equilibrium constants and salting out coefficient using classical thermodynamic approach. Thermodynamic parameters such as heat of reaction, Gibb's free energy change and entropy change were estimated by analysing the experimental data.

Publications

1. "Development of a continuous homogeneous process for denitration by treatment with formaldehyde", Satyabrata Mishra, Falix Lawrence, R. Srinivasan, N.K. Pandey, C. Mallika, S.B. Koganti and U. Kamachi Mudali, J. Radioanal. Nucl. Chem. 2010, 285, 687695.
2. "Development and characterization of porous silicon nitride tubes", Satyabrata Mishra, C. Mallika, P.K. Das, U. Kamachi Mudali and R. Natarajan, Trans. Ind. Ceram. Soc. 2013, 72, 52-55.
3. "Thermodynamics of solubility of tri-n-butyl phosphate in nitric acid solutions", Satyabrata Mishra, S. Ganesh, P. Velavendan, N.K. Pandey, C. Mallika, U. Kamachi Mudali and R. Natarajan, Adv. Chem. Engg. Research, 2013, 2, 55-60.
4. "Effect of temperature, concentration of acid and metal ions on the solubility of TBP in aqueous phase", Satyabrata Mishra, S. Ganesh, P. Velavendan, N.K. Pandey, C. Mallika, U. Kamachi Mudali and R. Natarajan, J. Radioanal. Nucl. Chem. (Communicated).
5. "Effect of metal ions and organics on chemical denitration of HLLW", Sanat Karmakar, Satyabrata Mishra, C. Mallika, U. Kamachi Mudali and R. Natarajan, J. Chem. Engg. Sci. (Communicated).
6. "Electrochemical divided cell design for radioactive environment", Satyabrata Mishra, Falix Lawrence, N.K. Pandey, C. Mallika, U. Kamachi Mudali and R. Natarajan, J. Appl. Electrochem. (To be communicated).
7. "A comparative study on the evolution of physiochemical properties and metal retention behaviour of thermally degraded TBP-Dodecane-HNCL/TBP-NPH-HNCL systems", Satyabrata Mishra, S. Joshi, N.K. Pandey, C. Mallika, U. Kamachi Mudali and R. Natarajan, Sep . Sci. Technol. (To be communicated).
8. "A systematic study on the effect of radiolysis in alteration of physiochemical and metal retention properties of TBP-Dodecane-FTNCL and TBP-NPH-HNO3 systems", Satyabrata Mishra, S. Joshi, N.K. Pandey, C. Mallika, U. Kamachi Mudali and R. Natarajan, Sep. Sci. Technol. (To be communicated).

Conference Proceedings

1. Satyabrata Mishra, Falix Lawrence, R. Srinivasan, N.K. Pandey, C. Mallika and S.B. Koganti, "Influence of surface area of anodes in electrochemical reduction processes and performance evaluation of an electroplated Ti anode", Proc. Discussion Meet on Electroanalytical Techniques and Their Applications (DM-ELANTE-2008), Munnar, Feb. 2008, Paper No. 15.
2. Satyabrata Mishra, Falix Lawrence, C. Mallika, S.B. Koganti and U. Kamachi Mudali, "Characterisation of reaction bonded silicon nitride tubes", 20th Annual Conf. of Indian Nuclear Society (1NSAC - 2009), organized by INS, IGCAR and BHAVINI, Chennai, Jan. (2010), p. 124.
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Enrolment No.	:	ENGG02200804028
Date of Award of degree	:	21.04.14
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	Corrosion Behaviour of Carbon Materials and Development of Ceramic Coatings on Graphite Crucibles for Molten Salt Based Applications

Abstract

To establish pyrochemical reprocessing plants for reprocessing of spent metallic fuelsof Fast Breeder Reactors with various unit operations it is necessary to identify, develop andqualify reliable corrosion resistant materials and coatings for service in molten LiCl-KCl saltand molten uranium environment operating between 773 to 1573 K. Carbon based materialsare proposed as candidate materials for salt purification and cathode processor crucibles,vessels and liners in pyrochemical reprocessing involving molten LiCl-KCl salt medium andmolten uranium. The present thesis work is focused on evaluation of materials and coatingsfor salt purification system crucible where molten LiCl-KCl salt will be handled and for thecathode processor crucible where the combined environment of 20 wt% molten salt, cadmium and molten uranium is present. To meet the requirement of pyrochemical reprocessing unit operations, the evaluation and performance of materials and coatings were studies in molten LiCl-KCl salt at 873 K for 2000h as well as in molten uranium at 1623 K. The corrosion behaviour of the carbon materials viz. low density graphite (LDG), high density graphite (HDG), glassy carbon (GC) and pyrolytic graphite (PyG) was investigated in molten LiCl- KCl electrolyte salt medium at 873 K for 2000 h under ultra high pure (UHP) argon atmosphere for selecting the material for salt purification crucible application. Morphological changes in the carbon materials exposed to molten LiCl-KCl salt revealed severe corrosion attack on LDG and HDG and the attack on GC was insignificant due to non-penetration of salt into GC. Removal of carbon particles and surface degradation were not found in PyG exposed to molten LiCl-KCl and these are observed in LDG and HDG. The corrosion resistance of carbon materials in molten LiCl-KCl salt at 873 K was observed to follow the order: LDG < HDG < GC < PyG.

Owing to its availability and economic viability, HDG is considered as one of the structural materials for salt purification system and as cathode processer crucible. The performance of HDG in molten LiCl-KCl salt clearly indicated that ceramic coatings are desirable on HDG components (crucibles) in order to protect them from corrosion attack by salt and molten uranium and to extend their service life and mechanical integrity at high operating temperatures. Hence, ceramic coatings of partially stabilized zirconia (PSZ) with NiCrAlY bond coat and top alumina-40 wt% titania (A40T) with bond coat of Cr3C2-NiCr and without bond coat were developed on HDG substrates by plasma spray process and these were evaluated for deploying these coated materials for crucible, liners and vessels applications in pyrochemical reprocessing. The ceramic coated HDG samples were exposed to molten LiCl-KCl salt for 2000 h at 873 K under UHP argon atmosphere and compatibility test with molten uranium at 1623 K for 20 min under UHP argon atmosphere. The unit operations of salt purification and cathode processor are batch processes in pyrochemical reprocessing. Hence, the durability of coatings developed on HDG substrate need to be evaluated. For this purpose, ceramic coated HDG samples were subjected to thermal cycling to understand the durability of the coatings. The molten salt tested carbon materials and ceramic coated HDG (as-coated and tested) samples were characterized by Scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDX), Atomic force microscopy (AFM), X-ray diffraction (XRD) and Laser Raman spectroscopy (LRS).

The A40T coating developed cracks and salt deposits were found after exposure to molten salt for 500 h and spallation of A40T coating occurred from HDG substrates after 2000 h of exposure with Cr3C2-NiCr bond coated as well as without bond coat. To improve the performance of A40T coating in molten salt, post treatments (annealing and laser melting) were performed. It is

evident from the results that denser and compact microstructure can be obtained by pulsed laser melting as compared to vacuum annealing of coatings. Laser melted A40T coatings were exposed to molten salt showed that the laser melted coatings exhibited better corrosion resistance owing to their fully dense top layer. The PSZ coated HDG exhibited excellent corrosion resistance in molten LiCl–KCl salt due to good adherence of the coating to the substrate even after 2000 h of exposure and no change in the morphology as well as in the phases of the PSZ coating was observed.

For selecting a coating for cathode processor crucible, the studies were carried out for testing the PSZ coated samples with molten uranium at 1623 K. A40T coating exhibited poor adhesion on graphite surface and spallation of coating was observed after compatibility test with molten uranium in addition to the adherence of uranium metal on the coating surface. The compatibility of molten uranium with PSZ coatings studies showed that PSZ coating protect the HDG, since the reaction products/layer observed on the surface of the coating was insignificant. A40T coated HDG with Cr3C2-NiCr and without bond coat samples were subjected to thermal cycling studies at 873 K exhibited complete coating spallation after 60 and 80 cycles respectively. The failure of A40T coating is due to the poor adhesion strength of the coating to the HDG substrates in both the cases. PSZ coated HDG subjected to thermal cycling studies at 873 and 1023 K showed that PSZ coating did not exhibit any failure of the coating even after 200 cycles and only network of cracks generated in the microstructures still resolved with stable tetragonal phase of the PSZ. The results of the studies reported in this thesis upheld the choice of HDG crucibles and PSZ coating on them for corrosion protection in molten chloride salt medium and molten uranium based on the performance in both the environments. Finally, PSZ coating was developed on engineering scale facility HDG crucibles for future studies at 1623 K to evaluate the combined (molten salt and molten uranium) environment effect on the coated crucibles.

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2. Jagadeesh Sure, A. Ravi Shankar, U. Kamachi Mudali, A Nowicki, Baldev Raj, Characterization of pyrolytic graphite exposed to molten LiCl-KCl salt, Surface Engineering 2013, 29, 28-33.
3. Jagadeesh Sure, A. Ravi Shankar, B.N. Upadhyay, U. Kamachi Mudali, Microstructural characterization of plasma sprayed Al2O3-40 wt.% TiO2 coatings on high density graphite with different post-treatments, Surface and Coatings Technology 2012, 206, 4741-4749.
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8. Jagadeesh Sure, A. Ravi Shankar, K. Thyagarajan, U. Kamachi Mudali, Molten salt corrosion behaviour of plasma sprayed alumina–40wt% titania coating on high density graphite in molten LiCl-KCl salt, Materials at High Temperatures (Revised manuscript under review).

9. Jagadeesh Sure, C. Mallika, Ambar Choubey, U. Kamachi Mudali, Corrosion behaviour of laser melted alumina-40 wt % titania coated high density graphite exposed to LiCl-KCl molten salt at 873 K- A microstructural study, Surface Engineering (Under review).
10. Jagadeesh Sure, A. Ravi Shankar, K. Thyagarajan, C. Mallika, U. Kamachi Mudali, Thermal cycling behaviour of plasma sprayed partially stabilized zirconia coatings on high density graphite substrate, Journal of Thermal Spray Technology (Under review).
11. Jagadeesh Sure, Ch. Jagadeeswara Rao, C. Mallika, U. Kamachi Mudali, Review on pyrolytic graphite for pyrochemical reprocessing application Transactions of Indian Institute of Metals (Manuscript under preparation).

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2. Jagadeesh Sure, A. Ravi Shankar, U. Kamachi Mudali, Characterization of plasma sprayed alumina-titania coating on high density graphite for pyrochemical reprocessing applications, Poster presentation at 1st International Conference on Recent Trends in Materials Science and Technology (ICMST), Indian Institute of Space Science and Technology, VSSC, Thiruvananthapuram, Oct (2010).
3. Jagadeesh Sure, A. Ravi Shankar, S. Ramya and U. Kamachi Mudali, Evaluation of corrosion behaviour of plasma sprayed partially stabilized zirconia coated and uncoated high density graphite in molten LiCl-KCl salt, Oral presentation at 25th International Conference on Surface Modification Technologies (SMT-25), University West, Throllhättan, Sweden, June (2011).
4. Jagadeesh Sure, A. Ravi Shankar, S. Ramya, U. Kamachi Mudali, Molten salt corrosion behaviour of partially stabilized zirconia coated high density graphite in LiCl-KCl medium, Oral presentation at 49th National Metallurgists' Day (NMD) and 65th Annual Technical Meeting (ATM), The Indian Institute of Metals, Shameerpet, Hyderabad, Nov (2011).
5. Jagadeesh Sure, A. Ravi Shankar, U. Kamachi Mudali, Laser surface melting of plasma sprayed alumina-titania coating on high density graphite, Poster presentation at International Conference on Advanced Materials (ICAM 2011), PSG College of Technology, Coimbatore, Dec (2011).
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9. Jagadeesh Sure, C. Mallika, U. Kamachi Mudali, Corrosion behaviour of carbon materials and development of ceramic coatings on high density graphite for molten salt application, Poster presentation at The International Corrosion Prevention Symposium for Research Scholars (CORSYM-2013), GRT Grand, Chennai, Feb-Mar (2013).
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11. Jagadeesh Sure, M. Mishra, M. Tarini, A. Ravi Shankar, N.G. Krishna, P. Kuppusami, C. Mallika, U. Kamachi Mudali, Microstructural characterization and chemical compatibility of pulsed laser deposited yttria coatings on high density graphite, The Sixth International Conference on Technological Advances of Thin Films and Surface Coatings (THINFILMS-2012), July 14-17th, 2012, Singapore Management University(SMU) at Stamford Road, Singapore.

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Title	:	Structural, Microstructural and Thermo-Physical Properties of Alkaline Earth Based Phospo-Silicate Glass/Glass-Ceramics

Abstract

Phosphate based glasses have low durability, but addition of silica can increase the stability of phosphate based glasses, which can lead to different applications such as an implant in biomedical or bonding of different materials. The high phosphate containing silicate glasses with different additives like iron oxide, ZnO and Ag have been investigated as prospective bio-materials. The glass/glass-ceramics with nominal compositions $34SiO_2$-(45-x)CaO-$16P_2O_5$-4.5 MgO-$0.5CaF_2$ -xFe_2O_3 (x = 5- 20 wt %), $25SiO_2$-$50CaO$-$15P_2O_5$-(10-x)Fe_2O_3-xZnO (x = 0-5 mol %) and $25SiO_2$-(50-x)CaO-$15P_2O_5$-$8Fe_2O_3$-2ZnO-xAg (x = 0- 4 mol %) were studied. It was found that the addition of iron oxide and zinc oxide modifies the structural, micro-structural properties. Iron oxide behaves as network modifier at low concentration and stabilizes the glass network at higher content. ZnO stabilizes the glass network when its content increases. In-vitro studies have shown the formation of bioactive layer after different time of immersion in SBF. The adhesion of polymer has been seen on the glass-ceramics when immersed in BSA, implying good biocompatibility. However, polymeric adhesion decreases with addition of ZnO. Antibacterial response of Ag containing glasses against with Escherichia coli (E. coli) was studied. The glass samples with 4 mol % Ag have shown effective antibacterial activity against E. coli. P_2O_5 can be useful as nucleating agent to avoid undesirable reaction at the metal glass interface. In a novel idea, glasses with low phosphate content have been formulated by the combined addition of P_2O_5 and BaO [$Ba_3(PO_4)_2$] to a base glass composition (mol%) $30SiO_2$-$20SrO$-$30BaO$-$10B_2O_3$-$5La_2O_3$-$5Al_2O_3$. The positive effect of $Ba_3(PO_4)_2$ incorporation on thermo-physical properties has been demonstrated by the decrease in softening temperature, enabling the seal fabrication (with Crofer-22APU) below 1000°C. Moreover, crystalline phases and TEC were found to be stable and compatible for sealing applications. The effects of P_2O_5 as a nucleating agent was found further

corroborated in the presence of V_2O_5. The V_2O_5 and P_2O_5 were found involved in the crystallization process of glasses with nominal composition (mol%) $27SiO_2$-23SrO-32BaO-$4Al_2O_3$-$10B_2O_3$-(4-x)P_2O_5-xV_2O_5.$BaSi_2O_5$,$BaAl_2Si_2O_8$, $Ba_{0.9}Sr_{0.1}Al_2Si_2O_8$ and Sr_2SiO_4 are observed as major crystalline phases. The addition of V_2O_5 has been found beneficial in glass formulation as the sealing temperature was reduced.

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a. Paper in Journals

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3. G. P. Kothiyal, M. Goswami, Babita Tiwari, K. Sharma, A. Ananthanarayanan, Lionel Montagne, J. Adv. Ceram. 1(2)(2012)110.
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12. G. P. Kothiyal, A. Arvind, R. Kumar, A. Dixit, Kuldeep Sharma, Madhumita Goswami, J. Phy. Conf. Series-2009. IOP Conf. Series: Mater. Sci. Eng. 2 (2009) 012005.

b. Paper in Conference/Symposium Proceedings

1. K. Sharma, A. Ananthanarayanan, G. P. Kothiyal, L. Montagne, F. O. Mear, G. Tricot, and B. Revel , European Fuel Cell - Piero Lunghi Conference & Exhibition, December 14-16, 2011, Rome, Italy
2. L. Montagne, F. Méar, S. Castanie, K. Sharma, G. P. Kothiyal, ICONSAT, January 21-26, 2012, Hyderabad, India.
3. K. Sharma, A. Dixit, A. Arvind, G. P. Kothiyal, Symposium on synthesis and Characterization of Glass and Glass-ceramics, July 7-8, 2010, CMET-Pune.
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5. K. Sharma, A. Dixit, Sher Singh Meena, S. M. Yusuf, A. Srinivasan, G. P. Kothiyal, Symposium on synthesis and Characterization of Glass and Glass-ceramics, July 7-8, 2010, CMET-Pune.
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Title	:	Twisted Conjugacy Classes in Lattices in Semisimple Lie Groups

Abstract

Let Γ be a group and let ϕ : Γ → Γ be an endomorphism. We define an action g.x := gxϕ(g−1), for g, x ∈ Γ, of Γ on itself. The ϕ- twisted conjugacy class of an element x ∈ Γ is the orbit of this action containing x. A group Γ has the R∞-property if every automorphism ϕ of Γ has infinitely many ϕ-twisted conjugacy classes. In this thesis we show that any irreducible lattice in a non-compact connected semisimple Lie group with finite center and having real rank at least 2 has the R ∞-property. We also show that any countable abelian extensions Λ of Γ has the R ∞-property when (i) the lattice Γ is linear, (ii) Γ is a torsion free non-elementary hyperbolic group. We also consider the R ∞-problem for S-arithmetic lattices.

Publications

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Name	:	**Surya Pratap Singh**
Enrolment No.	:	LIFE09200804011
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Title	:	Development of in vivo Raman Diagnostic Methodolgies for Oral Pre-Cancers and Cancers

Abstract

Oral cancer is the most prevalent cancer among Indian males. Long term tobacco habits are considered as major etiological factors. Subjectivity, time consumption are some of the well known limitations of the conventional diagnosis methods. The work reported in the thesis aims towards developing and evaluating potential of in vivo laser Raman spectroscopy methods for non-invasive and objective diagnosis of oral cancers and pre-cancers under clinical setting.

The first objective was to standardize data acquisition and analysis protocols on ex vivo oral tissues before initiating the in vivo studies. A total of 683 spectra from 36 pairs of biopsies were obtained. Lipid rich features were observed in normal spectra while tumor showed predominant protein bands. Correlation with histopathology suggests that misclassification between both

groups can be primarily attributed to the tissue heterogeneity. By acquiring spectra of intact and incised oral biopsies, it was demonstrated that morphological and architectural arrangements of different layers in a tissue contribute to the spectral signatures. Spectral features of normal and tumor tissues were also correlated with underlying biochemical composition. Area associated with protein (1450 cm^{-1} and 1660 cm^{-1}) and lipid (1440 cm^{-1}) bands were computed and correlated with biochemical estimation. Spectral parameters derived from curve resolved protein and lipid Raman bands were found to be highly correlating with biochemical measurements.

Following standardization of data analysis and acquisition protocols in vivo studies were undertaken as part of second objective. For the first time, we demonstrated the feasibility of acquiring good quality in vivo Raman spectra under clinically implementable time in Indian population. A total of 444 contralateral normal, 337 tumor and 206 premalignant spectra from 163 subjects were acquired. Mean and difference spectra suggest predominant lipid features in normal conditions while proteins are rich in tumors. Discrimination of premalignant conditions against closely associated habitual tobacco users was also demonstrated. Another in vivo study involving healthy controls, habitual tobacco users and non-tobacco cancer subjects was carried out, to evaluate potentials of RS in identifying histologically unrecognizable molecular changes that are indicative of neoplastic transformation. Findings suggest that 'cancer field effects' or 'malignancy associated changes' can be objectively identified and supports its potential to become a mass screening tool in public health programs.

In the third objective, a study on tongue cancer derived AW13516 cell-line was taken up to evaluate potentials of Raman spectroscopy in identifying minor changes associated with differential level of keratin expression. Spectral features are suggestive of differences in the protein content and secondary structures. Individual cell morphology was analyzed and findings suggest that vector control cells have more actin based filamentous protrusions and they are elongated in shape. However, cells in which Keratin 8 was knocked down show very few actin-based protrusions and have symmetric contracted epithelial appearance. Morphological differences were established by generating Raman maps of single cells. Different clusters corresponding to membranous, cytoplasmic, perinuclear and nuclear regions of the cell were obtained.

The reported thesis highlighted the efficacy of Raman spectroscopic methods in conjunction with multivariate analysis tools for unambiguous and non-invasive identification of normal and pathological conditions as well as the early invisible changes which may be an indicative of neoplastic transformation in oral cancers.

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1 Atul Deshmukh*, S.P.Singh*, Pankaj Chaturvedi, C. Murali Krishna, "Raman spectroscopy of normal oral buccal mucosa tissues: A study on intact and incised biopsies" J Biomed Opt16 (12), 2011 (*Equal contribution). (DOI: 10.1117/1.3659680.)

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Title : Photon Production and Forward-Backward Multiplicity Correlation in Alice at the LHC

Abstract

In this thesis an attempt has been made to measure the multiplicity and pseudoraidity distributions of the inclusive photons and forward-backward (F-B) multiplicity correlations of charged particles in ALICE at the LHC. Photon production has been studied in p-p and p-Pb collisions using the data from the Photon Multiplicity Detector (PMD) and the data from the ALICE central barrel (Time Projection Chamber (TPC) and Inner Tracking System (ITS)) has been used to study the F-B correlations in p-p collisions.

The first part of the thesis includes the detailed description of PMD, the testing of the PMD modules and extracting the photon signals using the experimental data and simulation. Multiplicity distribution and pseudorapidity density of incident photons at forward rapidities ($2.3 < n < 3.9$) have been presented in p-p collisions at $\sqrt{s}$ = 2.76 and 7 TeV with the expectation from different event generators like PYTHA Perugia - 0 and PHOJET. It is found that both the models underpredict the data. It is observed that the photon multiplicity distributions are well described by negative binomial distributions (NBD). It is shown that the increase in the average photon multiplicity as a function of beam energy is compatible with both a logarithmic and power law dependence. Limiting fragmentation behavior of photons has been studied. Preliminary results of pseudorapidity density of inclusive photons have been presented in p-Pb collisions at = 5.02TeV within $2.3 < n < 3.9$. The results are presented for minimum-bias as well as different centrality classes of p-Pb collisions with the expectation from the DPMJET event generator.

The second part of the thesis includes the study of the forward-backward multiplicity correlation in p-p collisions at $\sqrt{s}$ = 0.9, 2.76 and 7 TeV and the method for the study in heavy-ion collisions. The results have been presented for minimum bias p-p events within the acceptance of $|n| < 0.8$ and $0.3 < p_T < 1.5$ (GeV/c). Two separate pseudorapidity windows with a bin width of 0.2 to 0.8 rapidity units have been chosen symmetrically around n = 0. The multiplicity correlation strength has been studied as a function of n gap between the two windows as well as the width of these windows. It is observed that the correlation strength decreases with increasing n gap i.e. with increasing distance between two n windows and increases with the width of the each window. The results have been compared to different MC generators such as, PYTHIA Perugia - 0, PYTHIA Perugia - 11 and PHOJET. The relative correlation has been studied in terms of the ratio of the correlation strength of 7 TeV and 2.76 TeV with respect to 0.9 TeV and it is found to significantly increase with beam energy. Transverse momentum (p_T) dependence of the correlation strength has been studied. Method for the analysis of forward-backward multiplicity correlation in heavy-ion collision has been studied using the HIJING event generator. The results are presented for different centralities using two different methods. It is shown that the method, which takes into account the fluctuation in centrality selection, should be chosen to determine the forward-backward correlation strength in heavy-ion collisions.

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23. Transverse sphericity of primary charged particles in minimum bias proton-proton collisions at y^ = 0.9, 2.76 and 7 TeV Eur. Phys. J. C 72, 2124 (2012) (ALICE Collaboration)Production of muons from heavy flavour decays at forward rapidity in pp and Pb-Pb collisions at /sNN = 2.76 TeV

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4. Forward-backward multiplicity correlations in pp collisions in ALICE at 0.9, 2.76 and 7 TeV G. Feofilov, I. Altsybeev, V. Vechernin, Sudipan De, B. K. Srivastava Proceeding of Science (Baldin ISHEPP XXI) 075
5. Method for the study of forward-backward multiplicity correlations in heavy-ion collisions Sudipan De, B. K. Srivastava, T. K. Nayak Proceedings of the DAE Symp. on Nucl. Phys. 58 (2013) 776

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Abstract

In this thesis, we briefly discuss some theoretical shortcomings of the Standard Model (SM) and motivate the need for beyond the SM (BSM) physics. Many BSM extensions predict the existence of new heavy fermions with masses near the TeV scale. In this thesis we study the LHC phenomenology of two types of such new heavy fermions, namely the vectorlike quarks (VLQ) that arise in various warped extra-dimensional theories, and the color octet electrons (COE) that appear in some quark-lepton compositeness models. We review the construction of the original Randall-Sundrum model. We show how this model solves the gauge hierarchy problem of the SM. We also discuss how warped geometry can address the flavor hierarchy problem of the SM by allowing SM fermions into the bulk. We give the details of some warped models both without

and with custodial protection of the Zbb coupling that have been proposed earlier in the literature. For each of these models we carefully work out various Lagrangian terms in the mass basis relevant to the phenomenology we discuss in the thesis. We present the parameter choices, which we use for our numerical results, for the different warped-space models.
More than one heavy charge -1/3, 2/3 and 5/3 VLQs can be present in different warped-space models, and they can mix among themselves and the SM quarks. We explore the pair production channel for discovery of the new VLQs. However, in addition to pair production, we also look into some of their important single production channels since single production processes can give useful information about the electroweak nature of the underlying models. We compute the discovery luminosity and reach of the different VLQs at the LHC.

We discuss the LHC phenomenology of COE in an effective theory framework. We briefly discuss various preonic models of quark-lepton compositeness in which COE are present. We display the interaction Lagrangian of a generic COE and decay width of COE for different choice of compositeness scale. We have identified a new set of single production diagrams whose contribution is comparable to other dominant production channels of the COE. In a realistic computation, after parton showering and hadronization, it is very difficult to separate different production processes from each other. We implement a search method where the signal is a combination of pair and single production events. This method has potential to increase the LHC reach significantly. We compute the discovery lumonosity and reach of the COE at the LHC.

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Title	:	Molecular and Biochemical Studies of Aeromonas SPP

Abstract

Genus Aeromonas has emerged as an important human and fish pathogen. Detailed studies regarding the prevalence and characterization of Aeromonas from foods are lacking in India. A total of 154 food samples {sprouts (80), chicken (14) and fish (60)} were evaluated for the presence of Aeromonas. Higher prevalence and diversity of Aeromonas species was observed in

foods of animal origin (21.6%) as compared to plant origin (2.5%). Twenty-two Aeromonas isolates were identified till species level based on biochemical and molecular methods (16S rRNA and rpoD sequence analysis). These isolates were identified as A. salmonicida (6), A. veronii bv. veronii (4), A. caviae (3), A. hydrophila (2), A. veronii bv. sobria (2), A. jandaei (1), A. trota (1), A. sobria (1), A. allosaccharophila (1) and A. bivalvium (1). The rpoD gene was found to be a better phylogenetic marker than 16S rRNA gene, even at the intra-species level. Pulsed-field gel electrophoresis (PFGE) and whole cell protein (WCP) analysis showed high genetic diversity. Majority of these isolates were positive for virulence factors (virulence genes, extracellular enzymes and β-haemolysis) and showed marked resistance to commonly used β-lactam antibiotics. All Aeromonas isolates were very sensitive to gamma radiation, and radiation processing with 1.5 kGy was effective in achieving 5-log reductions in Aeromonas populations in mixed sprout, chicken and fish samples. Highly diverse and complex patterns of biofilm formation were observed in ten Aeromonas isolates under various abiotic stresses (nutrition, temperature, pH, NaCl and food preservatives). Biofilm formation under environmental stresses was found to be strain-specific phenomenon and no clear correlation was observed between the source of isolates and their biofilm forming ability. Aeromonas strains were very sensitive to different essential oils; minimum inhibitory concentration (MIC) values of clove, ajowain and cinnamon oils were ≤ 1 mg/ml. Significant expression of stress-response and virulence-associated genes was observed in A. hydrophila CECT 839^T and A331 strains under various stress conditions. Nutrient replenishment and deprivation significantly induced the housekeeping (rpoD and gapA), general stress regulator (uspA and rpoS) and virulence (aer) genes in A. hydrophila CECT 839^T and A331 strains, indicating their importance in regulating the survival and virulence of A. hydrophila under these conditions.

Publications

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Title	:	Synthesis and Characterization of Substituted Hydroxamic Acid and its Performance in the Separation and Purification of Pu and U

Abstract

Indian Nuclear Power program (INPP) has opted for the reprocessing of spent fuels from both thermal and fast breeder reactors, for the purpose of closing the nuclear fuel cycle. In the aqueous route for reprocessing of spent fuels, PUREX based solvent extraction process has been adopted for separating U and Pu from fission products. In the case of fuels discharged from fast reactors, problems are encountered due to high plutonium content in mixed carbide/oxide fuels, and high fission product inventory because of high burnups and these problems need to be addressed. For the separation of Pu and U (partitioning process), the salt-free acetohydroxamic acid (AHA) is considered to be a better partitioning agent, since it reduces the salt content in the liquid waste, thereby simplifying the waste treatment steps.

In the present work, AHA had been synthesized by a simple procedure and was characterized by IR, NMR and UV-Visible spectrochemical analysis. In the proposed method, hydroxylamine hydrate and acetic anhydride were used as the starting materials, without any catalyst. This facilitated the easy extraction of the compound formed and further crystallization at 0ºC after concentration. Characterization of the prepared compound indicated that its physical properties resembled closely to that of commercially available Sigma Aldrich (98% pure) product. The UV-Visible spectrophotometric method for the analysis of AHA was standardized based on the value of absorbance of Ferric ion - AHA complex and was adopted for the quantitative measurement of AHA in various stages of AHA utilization. Prior to employing AHA for uranium-plutonium separation, the reaction of AHA with metal ions in acid medium was studied to understand the mechanism for the formation of AHA-metal complex. It was observed that AHA reduces the metal ions exhibiting variable valency and the “nascent metal ion” produced complexes with AHA instantaneously. As such, AHA does not form any complex with metal ions in acidic medium. Experiments were conducted with radioactive plant solution for evaluating the efficiency of AHA in separating U and Pu. A comparison was made on the performance of uranous ions and AHA as reagents in uranium-plutonium partitioning process. Though uranous was found to be efficient in stripping plutonium, appreciable quantity of uranium was always present in the product stream, which requires extensive conditioning prior to reconversion process and ends up with uranium contaminated plutonium oxide product. On the other hand, AHA, as partitioning agent in nitric acid medium had led to product streams with very low uranium, resulting in pure plutonium oxide product. However, the number of stages required for complete stripping of plutonium was

higher with AHA as partitioning reagent when compared to uranous ions. Behaviour of the fission products Cs and Ru during partitioning process was compared for uranous and AHA. A uranium product contaminated with plutonium was purified using AHA and an optimized flow sheet was proposed.

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Abstract

A detailed study on the absorption of ultra-short, ultra-high intensity laser pulses and the corresponding x-ray emission from planar targets and various forms of nano-structures, has been carried out. As the absorption of the ultra-short intense laser pulses in smooth, planar targets is less, it is important to devise new techniques for increasing the laser energy coupling in high density matter. We have identified the conditions for maximizing absorption of intense ultra-short laser pulses in in situ formed nano-particles. The absorption was observed to exceed -70% in silver clusters produced in situ by sub-ns pulses. The high absorption resulted in a higher x-ray yield (in the >1 keV region) with a conversion efficiency of $8.5x10^{-2}$ %. This scheme further led to an order of magnitude enhancement of the x-ray emission in the water window spectral region (x-ray conversion of 0.54 % /sr) utilizing the in situ formed carbon clusters, as compared to that in a planar graphite target. Thus, it is demonstrated to be a simple, single step, cost effective method to obtain a high rep-rate, nearly debris free x-ray source. Using various nano-structures like spherical nanoparticles, nano-fibers, nano-rods, nano-tubes, and nano-holes, high laser energy absorption has been demonstrated, with near complete absorption in carbon nano-tubes. The theoretical consideration of the nano-particles has helped in understanding the role of target geometry in enhancement of the electric field, resonances, and the dynamics of the laser nano-structure interaction. We have analytically predicted multiple resonances in hollow nanostructure, which can facilitate continued occurrence of resonance. It was also shown that very efficient hot electron generation takes place in carbon nano-tube-coated targets, which results in an enhanced Ka line emission. Next, control of the size of the nano-particles is an

important aspect as the nano- particle properties are highly size dependent. It was observed that the size of the in situ formed nano-particles can be controlled easily by varying the incident laser pulse duration. A study of the nano-ripple formation in various semiconductors was also carried to study the dependence of the ripple width on the incident laser parameters, target material, band gap, and the ambient medium. The nano-ripple formation has been explained considering the transient metallic nature of the semiconductor surface on irradiation with a femtosecond laser pulse which excites surface plasmons, leading to the nano-ripple formation. The experimental observations help in identifying various conditions to grow the nano-ripples with controllable ripple period.

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2. Efficient keV x-ray generation from irradiation of in-situ produced silver clusters by Tksapphire laser pulses. U. Chakravarty, P.A. Naik, S.R. Kumbhare, and P.D. Gupta, J. Opt. Soc. Korea 13, 80, 2009
3. Formation of metal nano-particles of various sizes in plasma plumes produced by Tksapphire laser pulses. U. Chakravarty, P. A. Naik, C. Mukherjee, S.R. Kumbhare, and P. D. Gupta. J. Appl. Phys. 108, 053107, 2010
4. Enhanced soft x-ray emission from carbon nano-fibers irradiated with ultra-short laser pulses. U. Chakravarty, P. A. Naik, B. S. Rao, V. Arora, H. Singhal, G. M. Bhalerao, A. K. Sinha, P. Tiwari and P. D. Gupta Applied Physics B: Lasers and Optics , 103, 571, 2011
5. X-ray enhancement in a nano-hole target irradiated by intense ultra-short laser pulses. U. Chakravarty, V. Arora, J. A. Chakera, P. A. Naik, H. Srivastava, P. Tiwari, A.Srivastava, and P. D Gupta. J. Appl. Phys. 109, 053301, 2011
6. Nano-ripple formation on different band-gap semiconductor surfaces using femtosecond pulses. U. Chakravarty, R. A. Ganeev, P. A. Naik, J. A. Chakera, M. Babu, and P. D. Gupta. J. Appl. Phys. 109, 084347, 2011
7. Electric field enhancement at multiple densities in laser irradiated nano-tube plasma. U. Chakravarty, P.A. Naik, and P.D. Gupta Pramana J. Phys. 79, 443, 2012
8. Enhancement of K_a emission through efficient hot electron generation in carbon nano- tubes on intense laser pulse irradiation. U. Chakravarty, V. Arora, P. A. Naik, J. A. Chakera, H. Srivastava, A. Srivastava, G. D. Varma, S. R Kumbhare, and P.D Gupta J. Appl. Phys. 112, 053301, 2012
9. Estimation of electron density and temperature of semiconductor surfaces excited by ultra-short laser pulse U. Chakravarty, P.A. Naik , J.A. Chakera, A. Upadhyay and P.D. Gupta. Applied Physics A Materials Science & Processing DOI 10.1007/s00339-013-8063-y
10. Enhanced water window x-ray emission from in situ formed carbon clusters irradiated by intense ultra-short laser pulses. U. Chakravarty, B. S. Rao, V. Arora, A. Upadhyay, H. Singhal, P. A. Naik, J. A. Chakera, C. Mukharjee, and P.D. Gupta Applied Physics Letters 103, 054107, 2013

A.2 Thesis related papers presented in Conferences / Symposia

1. A novel method of intense keV x-ray generation from in-situ produced silver clusters using Ti: sapphire laser pulses. U Chakravarty, P.A Naik, R.A Khan and P.D. Gupta. DAE-BRNS National Laser Symposium, Vadodara, 2007 Awarded Best Poster Award by the "Indian Laser Association"\
2. Enhanced x-ray emission in water window region from ultra-short laser pulse irradiation of carbon nano-fibers. U. Chakravarty, P.A. Naik, B.S. Rao, V. Arora, H. Singhal, R.A. Khan, P.D.

Gupta, G.M. Bhalerao, A.K. Sinha, Fifth International Symposium on Modern Problems of Laser Physics, Novosibirsk, Russia, Aug. 2008\

3. Enhanced x-ray emission in water window spectral region from ultra-short laser pulse irradiation of carbon nano-fibers.,U.Chakravarty, P.A. Naik , B.S. Rao, V. Arora, H. Singhal, R.A. Khan, P.D. Gupta, G.M. Bhalerao and A.K. Sinha Fifth International Symposium on Modern Problems in Laser Physics, Novosibirsk, Russia, Aug. 2008
4. X-ray emission enhancement in various forms of carbon target under irradiation by ultra-short laser pulses. U.Chakravarty, P.A. Naik, R.K. Bhat, and P.D. Gupta, Fourth Asian Symposium on Intense Laser Science, Gwangju, Korea, Nov. 2008
5. Efficient keV x-ray generation from irradiation of silver clusters by Ti:sapphire laser pulses. U.Chakravarty, P.A. Naik, S.R Kumbhare, and P.D. Gupta , Fourth Asian Symposium on Intense Laser Science, Gwangju, Korea, Nov. 2008
6. Multiple electric field resonances in laser irradiated nano-shells. U. Chakravarty, M. P. Singh, P. A. Naik, and P. D. Gupta 26th National Symposium on Plasma Science & Technology, Patna, Dec.2008
7. A comparative experimental study of the absorption of intense, short laser pulses in plasmas formed by planar solids and nano-form matter. U. Chakravarty, P.A. Naik, J.A. Chakera, V. Arora, R.A. Khan, H. Srivastava, A. Srivastava, P. Tiwari, G.D. Verma, and P.D Gupta, DAE-BRNS National Laser Symposium, Mumbai, January, 2009.
8. X-ray emission enhancement in nano-hole alumina irradiated by intense Ti: sapphire laser pulses. U. Chakravarty, V. Arora, J. A. Chakera, P. A. Naik, FI. Srivastava, P. Tiwari, A. Srivastava, S.R. Kumbhare, and P.D Gupta. 24th National Symposium on Plasma Science & Technology, Hamirpur, Dec. 2009.
9. Metal nano-particle formation of various sizes in plasma produced by Ti:sapphire laser pulses. U. Chakravarty, P.A. Naik, R.K. Bhat, C. Mukherjee, and P.D. Gupta 24th National Symposium on Plasma Science & Technology, Hamirpur, Dec. 2009.
10. Enhancement of characteristic hard x-rays emission from an ultra-short pulse laser produced plasma source. V. Arora, U. Chakravarty, J. A. Chakera, P. A. Naik, S. R. Kumbhare, H. Srivastava, A. Srivastava, G. D. Verma, and P.D Gupta 24th National Symposium on Plasma Science & Technology, Hamirpur, Dec. 2009.
11. Electric field enhancement at multiple densities during hydrodynamic evolution of laser irradiated hollow dielectric nano-tubes. U. Chakravarty, P. A. Naik, and P. D. Gupta, International symposium on waves turbulence and coherent structure in plasmas, Gandhinagar, Feb 2010
12. Nano-ripple formation on different band-gap semiconductor surfaces using femtosecond pulses. U. Chakravarty, R. A. Ganeev, J. A. Chakera, M. Babu, P. A. Naik, and P. D. Gupta 19th DAE-BRNS National Laser Symposium , Indore, December, 2010.
13. Electric field resonances in laser irradiated nano-tubes. U. Chakravarty, P. A. Naik, and P. D. Gupta 19th DAE-BRNS National Laser Symposium , Indore, December, 2010.
14. Enhanced water window x-ray emission from graphite target by dual time delayed Ti:sapphire laser pulses. U. Chakravarty, B. S. Rao, V. Arora, H. Singhal, P. A. Naik, J. A. Chakera, and P.D. Gupta 25th National Symposium on Plasma Science & Technology, Guwahati, Dec. 2010.
15. Upshift of resonance density due to asymmetric expansion of laser irradiated nanorods. U. Chakravarty, P.A. Naik, P.D.Gupta 25th National Symposium on Plasma Science & Technology, Guwahati, Dec. 2010.
16. Resonant absorption and x-ray emission from nano-particles of various shapes irradiated by intense laser pulses. U. Chakravarty, P.A. Naik, V. Arora, J.A. Chakera, B.S. Rao, H. Singhal, S.R. Kumbhare, and P.D. Gupta Topical Conference on EM radiation interaction with atom molecule and cluster, Indore, March 2010.
17. A novel technique to obtain surface plasma electron density and temperature of semiconductor surfaces excited by ultra-short laser pulse. U. Chakravarty, P.A. Naik, J.A. Chakera and P.D. Gupta 27th National Symposium on Plasma Science & Technology, Puducherry, Dec.2012
18. Hole size effect in hard x-ray emission from intense laser irradiated nano-holes. U.

Chakravarty, V Arora, J. A. Chakera, P. A. Naik, H. Srivastava, P. Tiwari, A. Srivastava, and P.D Gupta 26th National Symposium on Plasma Science & Technology, Patna, Dec.2011. Awarded Best Poster Award by the "Plasma Science Society of India"

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Title	:	Synthesis of Functional Bodipy Molecules for Multiple Applications

Abstract

With the objectives of developing Bodipy-based materials for various applications several Bodipys were synthesized. The Bodipys, synthesized by replacing F atoms at the boron centre with a polyethyleneglycol (PEG) derivative as such, and in conjunction with introduction of meso-aryl group showed increased photostability than PM567, without compromising the lasing efficiency. Based on results of the theoretical calculations and pulse radiolysis studies, The improved photostability was explained in terms of reduced generation and reactivity with $^1O_2$. Subsequently, the concept of steric strain release was illustrated to formulate a new route for meso-functionalization of the Bodipy core overriding the acidity factor of per-methylated Bodipys.

For some biological studies, a panel of glycosylated Bodipys with red-shifted emission was synthesized for the first time. Bioevaluation of these molecules showed their i,pressive photo-toxicity without any dark toxicity and good bioavailability in human lung cancer A549 cells. The compounds induced cellular apoptosis via the extrinsic pathway, and are potential PDT agents. However, a diglycoside of dihydrostyryl Bodipy formed nano-hydrogel in aqueous EtOH and THF, and their size could be controlled by varying the water concentration.

In a radically different approach, a meso-alkenyloxyphenyl Bodipy-was grafted on Si to form σ–π monolayer that showed good current rectification due to a resonant transport between the Si conduction band and the HOMO of the π group. However, a self-assembly of the Bodipy, PM567 on the monolayer led to another type of device showing NDR behavior with good PVR (10-1000) with hysteresis.

Publications

Journal papers

1. K. K. Jagtap, # Neelam Shivran, # S. Mula,# D. B. Naik, S. K. Sarkar, T. Mukherjee, D. K. Maity and A. K. Ray Change of Boron Substitution Improves the Lasing Performance of Bodipy Dyes: A Mechanistic Rationalisation Chem. Eur. J. 2013, 19, 702-708. Equal contribution#
2. Vibha Saxena, P. Veerender, S.P. Koiry, A.K. Chauhan, D.K. Aswal, S. Mula, Neelam Shivran, S. Chattopadhyay and S.K. Gupta Borondipyrromethane (BODIPY) as Sensitizer for Dye sensitized solar cell. Proc. Am. Inst. Phys. 2012, 1451, 272-274. (Indian Vacuum Society Symposium on Thin Films: Science and Technology).
3. Neelam Shivran, S. Mula, T.K Ghanty and S. Chattopadhyay Steric Strain Driven Bodipy Functionalization Synfacts 2012, 8, 0036.
4. Neelam Shivran, S. Mula, T.K Ghanty and S. Chattopadhyay Steric Strain Driven Bodipy Functionalization Org. Lett. 2011, 13, 5870-5873. (Highlightedin Synfacts).
5. V. Saxena, S.P. Koiry, P. Veerender, Vasundhara, D.K. Aswal, S.K. Gupta, Neelam Shivran, S. Mula, S. Chattopadhyay, J.V. Yakhmi A simple photoelectrochemical cell using Fe^{+++}/Fe^{++} (aq) as redox couple. Proc. Am. Inst. Phys. 2010, 1313, 400-402. (International Conference on Physics of Emerging Functional Materials (PEFM- 2010)).
6. Neelam Shivran, M. Tyagi, P. Gupta, S. Mula, S. Chattopadhyay Synthesis and photodynamic activity of some glucose-conjugated BODIPY dyes (J. Med. Chem. communicated)

Conference papers

1. Shivran Neelam, Tyagi M., Mula S., Chattopadhyay S. A new tool for PDT: BODIPY-O-Glycosides. Sao Paulo Advanced School on Bio-organic Chemistry, Araraquara, Brazil, 30th June - 5th July, 2013, abstract no: OS-18.
2. Shivran Neelam, Mula S., S. P. Koiry, D.K.Aswal and Chattopadhyay S. Demonstration of Negative Differential Resistence (NDR) Behavior in Supramolecular Assembly of BODIPY Derivatives. Proc. 21st IUPAC International Conference on Physical Organic Chemistry (ICPOC-21), Durham, Royal Society of Chemistry, United Kingdom, September 9-13, 2012, abstract no: P-103.
3. Shivran Neelam, Mula S. and Chattopadhyay S. Synthesis and Photophysical Characterization of Bodipy Glycosides. Proc. 4th Interdisciplinary Symposium on Materials Chemistry (ISMC-2012), BARC, India, Dec. 11-15, 2012, abstract no: L-12
4. Shivran Neelam, Mula S., Jagtap K.K., Ray A.K. and Chattopadhyay S. Formulation of a Photo-stable Red-shifted BODIPY Laser Dye. Proc. DAE-BRNS 11th Biennial Trombay Symposium on Radiation & Photochemistry (TSRP-2012), BARC, India, Jan 4-7, 2012, abstract no: PC-126.
5. Shivran Neelam, Mula S., Jagtap K.K., Ray A.K., Dasgupta K. and Chattopadhyay S. Rational design of a new photostablepyrromethene laser dye. Proc. National Symposium on Radiation and Photochemistry (NSRP-2011), Jodhpur, India, March 10-12, 2011, abstract no: PC-83.
6. Saxena V., Koiry S.P., Veerender P., Vasundhara, Aswal D.K., Gupta S.K., Shivran Neelam, Mula S., Chattopadhyay S., Yakhmi J.V. A simple photoelectrochemical cell using Fe+++/Fe++ (aq) as redox couple. INTERNATIONAL CONFERENCE ON PHYSICS OF EMERGING FUNCTIONAL MATERIALS (PEFM-2010). Proc. Am. Inst. Phys. 2010, 1313, 400-402.
7. Shivran Neelam, Mula S., Koiry S.P., Aswal D.K. and Chattopadhyay S. Self- assembled BODIPY-bilayered silicon wafers with NDR property. Proc. DAE-BRNS 3rd International Symposium on Materials Chemistry (ISMC-2010), Mumbai, India, December 7-11, 2010, abstract no: D-14.
8. Jagtap K.K., Mula S., Shivran Neelam, Ray A.K. and Chattopadhyay S. BODIPY dye with improved photostablility and lasing efficiency. Proc. DAE-BRNS 10th Biennial Trombay Symposium on Radiation & Photochemistry (TSRP-2010), Lonawala, India, September 14-17, 2010, abstract no: PC-082.
9. Mula S., Jagtap K.K., Shivran Neelam, Ray A.K., Dasgupta K. and Chattopadhyay S. Rational Design of a new photostablepyrromethene (PM) laser dye. Proc. Ninth DAE-BRNS National Laser Symposium (NLS-09), BARC, Mumbai, India, January 13-16, 2010, abstract no: CP-33.

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Enrolment No.	:	LIFE09200604010
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Title	:	Role of Beta 1,6 Branched N-Linked Oligosaccharides in Regulating Key Cellular Processes Involved in Cancer Cell Invasion

Abstract

Expression of β1,6 branched N-linked oligosaccharides has been shown to correlate positively with invasiveness of several metastatic cancers. These are also expressed on the normal cells involved in invasive function, like trophoblast cells, activated granulocytes and macrophages. The study investigated the role of these oligosaccharides in regulating processes critical for cancer cell invasion by comparing invasive variant B16BL6 with its parent cell line B16F10 which differ in the expression of these oligosaccharides.

The first objective was to investigate the probable terminal substitutions on these oligosaccharides that might be providing optimum adhesion to matrix to be invasive. Alpha 2,6 linked sialic acids (SA) were found to be major terminal substitution that were associated with these oligosaccharides on B16BL6 cells. Inhibition of expression of ST6Gal-I, the enzyme that adds α2,6 linked SA on N-linked oligosaccharides decreased adhesion to both extracellular matrix (ECM) and basement membrane (BM) components fibronectin and matrigel, respectively. Substitution of α2,6 linked SA on these oligosaccharides was shown to be critical for influencing adhesion to matrices and thus invasion through matrigel, a reconstituted BM.

The Second objective was to investigate the role of β1,6 branched N-oligosaccharides in regulating another important aspect of invasion, that is matrix degradation. Although, the invasive variants did not differ in the basal secretion of MMPs, increased adhesion facilitated by these oligosaccharides induced secretion of MMPs and thus invasion. Inhibition of expression of these oligosaccharides inhibited adhesion and thus secretion of these enzymes. Further, the induction in MMP-9 secretion was shown to be due to increase in MMP-9 transcript. Besides, induction in MMP-9 secretion, enhanced expression of membrane tethered MT1-MMP also correlated with invasive potential of cells. Presence of these oligosaccharides on β1 integrin appeared to regulate the association of integrin receptors with MT1-MMP, thus coupling matrix degradation to movement.

Third objective was to investigate role of these oligosaccharides in regulating motility on ECM and BM components. Both fibronectin and laminin receptors were shown to carry these oligosaccharides. Glycosylation on integrin receptors was shown to regulate movement by modulating their association with respective tetraspanin enriched membrane microdomains. Presence of such oligosaccharides on laminin receptors α3β1 was shown to regulate its association with tetraspanin CD151 restraining cellular motility to promote invasion of the basement membrane (matrigel)

The reported thesis highlighted the complex mechanisms involved in cellular invasion and the role of β1,6 branched N-oligosaccharides in regulating them at multiple steps to achieve optimum invasion.

Publications

a. Journal Publication:

1. "Alpha 2,6 sialylation associated with increased β1,6 branched N-oligosaccharides influences cellular adhesion and invasion", AmitRanjan, Rajiv Kalraiya,J Biosci., December 2013, 38(5), 1-10 (DOI10.1007/s12038-013-9382-z).
2. "Glycosylation of the laminin receptor (α3β1) regulates its association with tetraspanin CD151: impact on cell spreading, motility, degradation and invasion of basement membrane by tumor cells",AmitRanjan, Sanjay M. Bane,Rajiv Kalraiya Experimental cell research, 1 April 2014, Volume 322, Issue 2, Pages 249–264 (DOI 10.1016/j.yexcr.2014.02.004).

b. Conference Publication:

1. "Glycosylation of laminin receptor integrin (α3β1) regulate their association with tetraspanin CD151 and thus motility/invasion on basement membrane component (matrigel)",AmitRanjan, Rajiv Kalraiya Glycobiology,(2012) 22(11): 1487-1661 doi:10.1093/glycob/cws127 (abstract published).

c. Journal Communicated:

1. "Mechanisms of matrix remodeling adopted by melanoma cells selected specifically for invasive characteristics",AmitRanjan, Rajiv Kalraiya and is under review in BioMed Research International.

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Enrolment No.	:	CHEM07201004001
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Title	:	N-Confused Porphyrin Derivatives : Syntheses Tautomeric Existence, Exchange, Aggregation Properties and Photodynamic Therapy

Abstract

This chapter describes the synthesis, spectral and structural characterization, solvent dependent tautomeric existence and exchange of a novel octa-hydroxy N-confused porphyrin derivative; meso-Tetrakis(3,5-dihydroxyphenyl)N-Confused Porphyrin (NCPH). The tautomeric existence and exchange of NCPH was investigated through various spectroscopic techniques such as UV-Vis, fluorescence and FT-IR spectroscopy in different polar protic and aprotic solvent combinations. A combination of DMSO/ACN, DMSO/H2O, MeOH/ACN and MeOH/H2O were used for the investigations. Solvent driven aggregation in these combinations was also monitored through scanning electron microscopy (SEM) and atom force electron microscopy (AFM) analysis. The morphological features observed in the different solvent combinations was explained on the basis of difference in the hydrogen bonding formation possible due to the existence of different tautomeric forms in the particular medium. Further, the role of anions in determining the morphology during aggregation was studied.

Publications

a) Published

1. 9,10,19,20-Tetraarylporphycenes: K. S. Anju, S. Ramakrishnan, Ajesh P. Thomas, E. Suresh, and A. Srinivasan, Org. Lett. 2008, 10, 5545-5548.
2. Calix[n]metallocenyl[m]phyrins (n = 1, 2 and m = 2, 4): aryl vs. alkyl: S. Ramakrishnan, K. S. Anju, Ajesh P. Thomas, E. Suresh, and A. Srinivasan, Chem. Commun. 2010, 46, 4746-4748.
3. Calix[2]-m-benzo-[4]phyrin with Aggregation-Induced Enhanced Emission Characteristics: Application as Hg2+ Chemosensor: P. S. Salini, Ajesh P. Thomas, R. Sabarinathan, S. Ramakrishnan, K. C. Gowri Sreedevi, M. L. P. Reddy, and A. Srinivasan, Chem. Eur. J. 2011, 17, 6598-6601.
4. 5,5-Diaryldipyrromethanes: syntheses and anion binding properties: K. C. Gowri Sreedevi, Ajesh P. Thomas, P. S. Salini, S. Ramakrishnan, K. S. Anju, M. G. Derry Holaday, M. L. P. Reddy, C. H. Suresh, and A. Srinivasan. Tetrahedron Lett. 2011, 52, 5995-5999.
5. 4,4,9,9-Tetraphenyl pyrroloindolizine: A Structural Analogue of Calix[2]pyrrole: K. C. Gowri Sreedevi, Ajesh P. Thomas, S. Ramakrishnan, P. S. Salini, M. G. Derry Holaday, M. L. P. Reddy, and A. Srinivasan. Org. Biomol. Chem. 2012, 10, 3600- 3605.
6. *meso-Tetrakis(p-sulfonatophenyl) N-Confused Porphyrin Tetrasodium Salt: A Potential Sensitizer for Photodynamic Therapy: Ajesh P. Thomas, P. S. Saneesh Babu, S. Asha Nair, S. Ramakrishnan, Danaboyina Ramaiah, T. K. Chandrashekar, A. Srinivasan and M. Radhakrishna Pillai. J. Med. Chem. 2012, 55, 5110-5120.
7. ansa-Ferrocene-Incorporated Calixpyrroles and Calixphyrins: Syntheses and Spectral/Structural Characterization. S. Ramakrishnan, K. S. Anju, Ajesh P. Thomas, K. C. Gowri Sreedevi, P. S. Salini, M. G. Derry Holaday, Eringathodi Suresh, and A. Srinivasan. Organometallics 2012, 31, 4166-4173.
8. *meso-Tetrakis(3,5-dihydroxyphenyl)N-Confused Porphyrin: Influence of polar protic and aprotic solvents in tautomeric existence, exchange and morphology. Ajesh P. Thomas, K. C. Gowri Sreedevi, B. Adinarayana, S. Ramakrishnan, and A. Srinivasan. RSC Adv. 2013, 3, 16967-16972.

*Pertaining to thesis

b) Communicated

1. Photoenolization of Diformyl Diaryldipyrromethane via ESDPT to Result in "Turn On" Fluorescence. K. C. Gowri Sreedevi, Ajesh P. Thomas, K. H. Aparna, Renuka Pradhan, M. L. P. Reddy, U. Lourderaj, and A. Srinivasan. Chem. Sci.

c) Manuscript under preparation

1. *Anion Induced Aggregation of meso-tetrakis(3,5-dihydroxyphenyl)N-Confused Porphyrin.
2. *Photodynamic Therapeutic application of meso-tetrakis(3,5-dihydroxyphenyl)NConfused Porphyrin.
3. *Morphological changes of free base and Ag(III) complex of long chain substituted derivatives of N-confused porphyrin.

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Title	:	Azimuthal Anisotropy Measurements for Identified Particles Produced in Au + Au Collisions At ÖsNN = 7.7-200 GeV

Abstract

The quantum chromodynamics (QCD), a theory of strong interaction between quarks and gluons, predicts that at very high temperature and/or high density quarks and gluons will be no longer confined within the hadrons [1]. This de-confined state is known as Quark-Gluon-Plasma (QGP). It is believed that just after Big-Bang the universe was consisted of free quarks and gluons. The main aim of the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory (BNL) is to create such de-confined state in laboratory and measure its properties.

After observing the clear signatures of the formation of QGP matter in Au+Au collisions at centre-of-mass energy (^/s_{NN}) of 62.4 and 200 GeV, attempts are being made to vary the colliding beam energy and to search for the transition region in terms of colliding beam energy between the partonic and/or hadronic dominant interactions in the QCD phase diagram. This is one of the main goals of the Beam Energy Scan (BES) program at RHIC [2]. In this program study of azimuthal anisotropy (known as elliptic flow) of produced particles will play a crucial role, since it is sensitive to the early dynamics of system created in the heavy-ion collision [7]. At top RHIC energy in Au+Au collisions, 0 meson has played an important role to establish that matter formed in such collisions is partonic i.e de-confined phase of quarks and gluons [36, 5]. Due to the small hadronic interaction cross-section, the yield and elliptic flow of the 0 meson are primarily controlled by the partonic interaction in the relativistic heavy-ion collisions [6, 17]. Therefore study of 0 meson will be the key measurement at RHIC BES program.
This thesis includes the study of elliptic flow of 0-meson and inclusive charged hadrons in Au+Au collisions at RHIC energies (^/s_{NN} = 7.7-200 GeV) in STAR experiment. The measurement of transverse momentum spectra of 0 meson at RHIC BES energies (Vs_{NN} = 7.7-39 GeV) has been presented. It also includes systematic measurement of centrality dependence of multi-strange hadrons (0, 5, and G) v_2 in Au+Au collisions at ¥/s_{NN} = 200 GeV. In addition, various models (Transport and Hydro) have been used to explain the experimental data. The content of this thesis is as follows. We will present the beam energy dependence of invariant yield and elliptic flow (v_2) of 0 meson in Au+Au collisions, data collected in the years 2010 and 2011 by the STAR experiment. The observed number-of-constituent quark (NCQ) scaling of identified hadrons v_2

was considered as signature for the formation of de-confined matter [8]. This NCQ scaling, mainly for multi-strange hadrons (0, S and Q), has been considered as a necessary signature for the formation of QGP [6, 17, 9]. In this thesis NCQ scaling of 0-meson v_2 will be presented for different beam energies to search for the turn-off of the QGP signature.

The nuclear modification factor (R_{eP}), defined as the particle yields in central nucleus- nucleus collisions to those in peripheral collisions, is also an important observable for studying QGP. For the QGP state, Rep is expected to be less than unity at the high p_T due to energy loss of high-p_T partons in the dense medium created in central collisions [12]. In addition, R_{eP} of identified hadrons shows particle type dependence (i.e baryon-meson separation) at intermediate p_T similar to v_2. To confirm this baryon- meson separation, 0 meson is considered as an essential probe, since it is a meson but it is has a mass comparable to the mass of the lightest baryons (such as proton). The measurement of 0-meson R_{eP} as a function of p_T for different centre-of-mass energies will be presented in this thesis.
We will also discuss particle ratio to shed light on 0-meson production mechanism in the heavy-ion collisions. The ratio of yield of the 0 meson to the yield of the kaon, N(0)/N(K), can be used to determine whether kaon coalescence is the dominant process for 0-meson production. The ratios N(0)/N(K) as function of collision centrality and centre-of-mass energy will be shown. The ratio of yield of the Q baryon to the yield of the 0 meson, N(Q)/N(0), are also observed to be sensitive to the particle production mechanism. At ^s_{NN} = 200 GeV, the ratios N(Q)/N(0) can be well explained by the quark recombination model for particle production [12, 11]. In this thesis, we will present the N(Q)/N(0) as function of p_T for various new beam energies in RHIC BES program.

In addition, we will explore the early dynamics of the system created in the heavy-ion collision by studying the elliptic flow of charged hadrons. In this thesis the measurement of inclusive charged hadron v_2 as function of transverse momentum, collision centrality and beam energy will be shown. These measurements will be compared to various models calculations and results from top RHIC and LHC energy.

Like 0 meson, other multi-strange hadrons i.e. S and Q also have small hadronic interaction cross sections and they freeze-out close to the quark-hadron transition temperature predicted by lattice QCD [13, 14, 15, 16]. Hence, the multi-strange hadrons are expected to provide information from the partonic stage of the evolution in the heavy-ion collisions. Due to limited statistics, from the earlier measurements on v_2 of multi-strange hadrons at RHIC, it was not possible to make strong physics conclusions. With high statistics data set collected by STAR experiment at top RHIC energy in the years 2010 and 2011, it is now possible to have high-precision measurements of multi-strange hadrons v_2. In this thesis we will present systematic measurements of centrality dependence of multi-strange hadrons v_2. Number-of-constituent quark scaling will be presented for different collision centrality classes to see how the partonic collectivity changes with different system size. Other possibility is to study the effect of the late-stage hadronic re-scattering on v_2 low p_T. Initial simulations using a hybrid model (Hydro+Cascade) showed that the usual mass ordering trend of $v_2(0) < v_2(p)$ will be reversed due to the late-stage hadronic re-scattering [16]. In this thesis we will investigate this effects by comparing v_2 of proton and 0 meson at low p_T in experimental data.

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Title	:	Probing of Polymer-Surfactant Interactions at Interfaces Using Light Scattering, Force Measurement and Rheology

Abstract

The main objectives of this thesis are (i) to get insight into the polymer-surfactant interaction at liquid-liquid interfaces and its consequences on the stability and rheological properties of liquid-liquid dispersions (ii) to investigate the role of surfactants and nanoparticles on self assembly and templating properties of triblock copolymers respectively. The competitive adsorption studies of polymer and surfactant at oil-water emulsion interface shows that the hydrodynamic diameter remains unchanged at low surfactant concentrations, but it increases dramatically above a critical aggregation concentration. The force measurement results show that at low surfactant concentrations, the interaction of surfactant monomers with the adsorbed polymers at droplet interface drastically changes polymer conformation and the onset of repulsion between the droplets. The phase contrast optical microscopic images of emulsion droplets preadsorbed with polymers of higher molecular weight show a systematic increase in the floe size on increasing surfactant concentration due to binding of polymer-surfactant complexes on several droplets. The zeta potential of the droplets increases on increasing ionic surfactant concentration due to preferential adsorption of surfactant at the oil-water interface.

The effects of interaction of surfactants on the self-assembly of a triblock copolymer (pluronic FI08) in aqueous solution shows that the addition of SDS in pluronic solution leads to a dramatic reduction in the viscoelastic properties, while it remains almost unaffected with CTAB and NP9. The two orders of magnitude decrease in the elastic modulus in the presence of SDS indicates a soft solid-like microstructure formed by aggregating self-assembled triblock polymers. The results suggest that the microstructure and elastic properties of block copolymer micelles can be tuned by varying the concentrations of ionic surfactant that enhances their potential in applications as nanocarriers for drug delivery systems. The addition of Fe3C>4 nanoparticle in a weak template of pluronic FI08 shows a decrease in the onset of gelation temperature and dramatic alteration in the viscoelastic moduli. The SAXS measurement shows that the intermicellar spacing of the supramolecular structure of pure pluronic FI 08 is — 16.5 nm and the supramolecular structure is destroyed when nanoparticles and surfactants are incorporated in it. These findings show that the thermogelation is due to the clustering of nanoparticles into a fractal network rather than close-packed FI08 micelles.

The main findings of the thesis work are as follows: (i) Lower molecular weight polymers with

suitable amount of ionic surfactants can synergistically enhance stability of formulations, while longer chain polymers induce flocculation, (ii) The percolation transition temperature T_p of triblock polymer in presence of ionic and nonionic surfactants is found to decrease with volume fraction of polymers, irrespective of the nature of surfactant used. The decrease in T_p with volume fraction of the triblock polymer-SDS mixed system is much slower compared to pure, cationic, and nonionic cases, (iii) The addition of nanoparticles and surfactant to triblock copolymer leads to a dramatic alteration in the viscoelastic properties. In summary, association of polymer, surfactant and nanoparticles can lead to several interesting phases and properties that can be exploited for practical applications such as stabilization of dispersions, rheology modification of dispersions and templating of nanoparticles.

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2. India-Brazil-South Africa Nanotechnology School on Advanced Materials (organized by IGCAR, Kalpakkam) held in Mahabalipuram, India during 22-26 February, 2010

   Poster presentation: Polymer-surfactant complexation on nano-droplets , J.S. Nambam & John Philip

   International Conference on Nanoscience and Technology held in Hyderabad, India (during 20-23 January, 2012 j Poster presentation: Triblock Copolymer-Iron Oxide Nanocomposite , J.S. Nambam & John Philip

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Title	:	Study and Characterization of Electron Cyclotron Resonance Plasma as an Ion Source

Abstract

In this thesis work, an electron cyclotron resonance ion source (ECRIS) has been designed, fabricated, and its subsystems have been individually characterized. From this source, a proton beam has been extracted and characterized, to be used as an injector for a CW proton accelerator.

The major components of the ECRIS are : microwave system, plasma chamber, vacuum system, electromagnets, high voltage insulator dome, ion beam extraction electrodes, plasma diagnostics and ion beam characterization devices. The microwave system consists of a magnetron source at

2.45 GHz frequency, capable of delivering 2 kW CW power, an isolator with water load, a directional coupler, a triple stub tuner, a high voltage break, a microwave window, and a microwave launcher. All these components, except the magnetron source, have been designed using Microwave Studio software, and after their fabrication, the system was characterized with vector network analyzer at low power and with a 2 kW glass water load at high power. The electromagnets, consisting of three-solenoid coils, have been designed using Poisson software, and after fabrication, characterized with a Hall probe. A field of 875 G was produced to satisfy the resonance condition at 2.45 GHz microwave frequency. The use of three coils provides a flexibility to work in off-resonance, flat, and mirror magnetic field configurations as per user requirement of singly or multiply charged ions. The argon, nitrogen, and hydrogen plasma was created with 300-1000 W of microwave power at a gas pressure of 10^{-5}-10^{-3} mbar. The plasma was characterized for its parameters like plasma density and electron temperature with an indigenously developed Langmuir probe. Three-electrode geometry was designed using IGUN software, fabricated, and integrated with the source for the extraction of proton beam. A proton beam current of 8 mA at 24 keV beam energy was measured using a Faraday cup. To characterize the charge states and energy distribution of the extracted ion beam, a Thomson parabola ion spectrograph was used. The results confirmed the existence of only protons, as no traces of any other hydrogen species (H_2^+ or H_3^+) from the plasma could be recorded.

In addition to the above work, this thesis also includes the measurement of the characteristics x-rays produced using argon/ hydrogen/ nitrogen ion beams impinging on a copper target. The bremsstrahlung continuum was also seen along with the characteristics copper K-a and K-(3 lines. As a demonstration of an application of the ECRIS, a titanium film was deposited on a glass substrate, using ECR argon ion beam bombarding a titanium target. The film was analyzed using standard techniques like x-ray reflectivity and atomic force microscopy.

The future goal is to upgrade this system to extract up to 30 mA proton beam current at 50 keV beam energy as an injector for a proton linac.

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Title	:	Thermodynamics of Ion Interaction in Solvent Extraction

Abstract

When an electrolyte is dissolved in water, it dissociates into cations and anions, which will be surrounded by water molecules as well as the counter ions and the electrolyte solution will no longer behave as an ideal solution. Nonideality in electrolyte solutions is attributed mainly to the interactions of water–ion and ion–ion. Thermodynamic properties, including activity coefficients at infinite dilution and other thermophysical and volumetric properties find application in the development of reliable predictive models for systems containing aqueous solutions

In the present thesis work, the ionic interactions have been investigated by measuring the half cell potentials of aqueous solutions of nitrates and chlorides of sodium and potassium by ISE meter and the results obtained were substituted in the Nernst equation to calculate the single ion activity coefficients. Activities of cations and anions were measured independently; the data generated were reliable as they could be reproduced reasonably well within the mean ionic activity coefficients.

Relative densities, refractive indices and viscosities have been measured for selected aqueous ionic systems and molecular liquids. These measurements were used to calculate various volumetric and excess properties. Density of aqueous solutions of sodium nitrate was measured from 293.15 to 343.15 K at 0.1 MPa pressure using Anton Paar DMA-5000 vibrating tube densitometer. These data were utilised to validate the data analysis programme at 298.15 K and at all other temperatures. Density and refractive index of several aqueous rare earth and fission product nitrates have been reported at 298.15 K and 0.1 MPa. Apparent molal volume, partial molal volume of the solvent, coefficient of thermal expansion etc. were calculated and discussed in terms of ionic contribution. The same procedure was extended for the temperature range

293.15 - 343.15 K and the effect of temperature on structural interaction has been evaluated. Using Hepler's assumption, structure maker and breaker behaviour has been predicted.

The density, refractive index and viscosity of molecular liquids like poly(ethylene glycol) (PEG) and 1-hexyl-3-methyl imidazolium bromide ([HMIm]Br) were also measured at 298.15 K and 0.1 MPa. Apparent molal volume was computed and compared with Masson's correlation to estimate apparent molal volume at infinite dilution. These properties at infinite dilution were used to explain structural interaction. These properties were also estimated in the temperature range 293.15 - 343.15 K for pure and aqueous solutions of PEG-200 and PEG-400. Coefficient of thermal expansion, variation in the second derivative of volume with temperature at constant pressure, excess volume, excess refractive index, and excess viscosity have been predicted and discussed in terms of structural interaction. Water activity and vapour pressure values have been reported for the ionic liquid [HMIm]Br.

This thesis also attempts to model the temperature and concentration dependence of the reported thermophysical properties of each system investigated using an equation of state, commonly referred to as the 'density model'. Wherever possible, the results of this model have been compared with those results from models reported in the literature.

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3. Debasmita Dash, S. Kumar, C. Mallika, U. K. Mudali, "Density, viscosity, refractive index, volumetric and excess properties of binary mixtures of poly (ethylene glycol) and water at 298.15 K and 0.1 MPa", Int. J. Thermophys. (Under review).
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1. Debasmita Dash, S. Kumar, C. Mallika, U. K. Mudali, "Volumetric properties of aqueous solutions of rubidium, strontium, samarium, yttrium, lanthanum, europium, praseodymium, and gallium nitrate at 298.15 K", Chemistry Research Scholar Meet (CRSM-2011), Kalpakkam.
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Title	:	Development and Implementation of the Trigger System for the Ino-Ical Detector

Abstract

The elusive neutrino has always perplexed the scientific community. The desperate attempt by Pauli in postulating its existence, followed by experimental discovery, to save the laws of conservation of energy and momentum in nuclear β-decay, bear testimony to this fact. Subsequent experiments like, Homestake, Sudbury Neutrino Observatory (SNO), Super-Kamiokande and KamLAND, which have studied neutrinos produced from various sources, provide concrete evidence in support of neutrino mass through the detection of neutrino oscillations. This serves as the first indication of the Physics beyond the Standard Model. Neutrino has also emerged as an excellent probe in comprehending the underlying laws of nature in particle physics, nuclear physics, astronomy and cosmology. In this context, a multi-institutional venture, called the India-based Neutrino Observatory (INO), has been initiated in India to participate in this exciting area of experimental particle physics by building a world-class underground facility for studying neutrinos.The INO collaboration has proposed to build a 50 kton magnetized Iron Calorimeter (ICAL) detector to study atmospheric neutrinos and to make precision measurements of the neutrino oscillation parameters. The detector will look for muon neutrino induced charged current interactions using magnetized iron as the target mass and around 28,800 Resistive Plate Chambers (RPCs) as sensitive detector elements. A magnetic field of 1.3 T will be used to discriminate between neutrino and anti-neutrino interactions, which equips the ICAL detector with the unique capability of determining the neutrino mass hierarchy. The extremely low rate of neutrino interactions necessitates the trigger scheme for such an experiment to achieve an optimization of the detection efficiency of the desired events and the chance trigger rates. It should also ensure feasibility of hardware implementation considering the vast volume of the detector. The development, validation and implementation of the ICAL trigger system, which satisfy these criteria, are documented in this thesis.

The design of the trigger scheme for the ICAL detector consists of a distributed and hierarchical architecture. The detector module is logically sub-divided into identical segments for the purpose of trigger generation. The segment dimensions are chosen considering the expected hit pattern of the events of interest, the associated chance trigger rates and the feasibility of implementation. Pre-trigger signals produced at the RPC level are combined together to generate a local trigger at the segment level, which in turn initiates a global trigger signal to invoke the data acquisition system to record the event data.The associated chance trigger rates have been calculated for different segment dimensions and for different sets of trigger criteria and are found to be negligible for an optimal combination of the trigger parameters. A simulation framework is developed to estimate the trigger efficiency of the scheme for the events of interest for the ICAL detector. The results ensure that substantially high detection efficiency can be obtained for the desired events under the proposed trigger scheme. The hardware implementation of the trigger scheme is initiated by designing an FPGA-based trigger module using the look-up table based technique. The module has delivered satisfactory performance in the prototype detector with negligible spurious trigger rate and trigger inefficiency. This ensures that such technique can be successfully and reliably employed in designing the ICAL trigger system. The overall layout for the implementation of the proposed trigger scheme for the ICAL detector has been devised and the trigger latency is estimated. A study is undertaken to ascertain the reliability of LVDS standard in transmitting the trigger signals for the ICAL detector. A technique for calibrating the delay offsets associated with the return-path of the trigger signal is proposed. The designs of the trigger boards are conceived and appropriate design components have been selected.

The work reported here has thus facilitated the evolution of the ICAL trigger system from the conceptual stage up to the board-level design.

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2) B. Satyanarayana, S. Dasgupta, S. Dhuldhaj, N. Mondal, P. Nagaraj, S. Rao, D. Samuel, M. Saraf, R. Shinde, S. Upadhya, V. Chandratre, V. Salodia, P. Saxena, M. Tewani, S. Saha, Y. Viyogi, "Electronics and data acquisition systems for the RPC based INO ICAL detector", In proceedings of XI Workshop on Resistive Plate Chambers and Related Detectors, POS(RPC2012)042.
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Title	:	Host-Pathogen Interactions of Different Strains of Mycobacterium Tuberculosis

Abstract

Tuberculosis (TB), the most prevalent chronic infectious disease in the world, causes 1.4 million deaths each year including nearly 50,000 deaths in India. The highly variable outcome of Mycobacterium tuberculosis (MTB) infection is determined by the battle between the host

immunity and the virulence of the MTB strain. Influence of MTB genomic diversity on disease outcome is still unexplored. In view of this the main objective of the of the study was to evaluate the effect of genetically diverse strains of MTB on in vivo as well as in vitro host responses.

Three different clinical isolates of MTB from three different lineages were selected for the study and were used for ex vivo as well as in vivo infection experiments. The strains were further characterized on the basis of TbD-1 and MIRU-VNTR loci and their drug susceptibility. The ex vivo infection study was carried out in THP-1 and RAW264.7 cells, as well as in primary cells, monocyte derived macrophages (MDM) and monocyte derived dendritic cells (MDDC), isolated from blood of healthy individuals. Initially, interactions between host and pathogen were monitored in terms of phagocytosis, intracellular growth of Mycobacteria, induction of proinflammatory cytokines, chemokines, and reactive oxygen/nitrogen species and apoptosis in THP-1 cells. Induction of proinflammatory cytokines followed a particular pattern for a single clinical isolate, in ex vivo experiments and the pattern was unchanged in different host cells. It was observed that the ancient EAI-5 strain from lineage-1 induced significantly higher proinflammatory response in the host compared to modern clinical isolates, as marked in earlier studies. On the other hand, modern Beijing strain from lineage-2 consistently induced low levels of proinflammatory cytokines and IL-10 according to its known lineage characteristic. Further, LAM-6 and H37Rv both belonging to lineage 4, showed similar proinflammatory responses. Similar interplay of different immune interactions was also clearly observed in the BALB/c model of TB following aerosol infection.

Overall, it was noticed that there existed a lineage specific cytokine induction pattern throughout ex vivo and in vivo infections as reported in previous studies and interestingly these patterns were not influenced by the drug resistant status of the strains. Strain specific apoptotic response was observed only for virulent strains. A positive correlation was observed between phagocytic index for '>10 bacilli/cell' and the percent apoptosis after five and six days of infection. It was evident that pro-inflammatory cytokines and initial higher accumulation of bacilli inside the host cell were the two determining factors for host cell apoptosis.

The present study is the first of its kind also because all the important parameters of immune interactions were monitored in hosts infected with highly drug resistant, well characterized MTB clinical isolates from distinct lineages in a single study. It illustrated lineage-specific patterns of innate immune responses induced by the strains of different genotypes in ex vivo and in vivo conditions. Such responses may reflect the differential survival strategies employed by clinical isolates to subvert the host immunity.

Publications

a. Published:

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b. Manuscript under preparation:

1) Mycobacterium tuberculosis strains from modern and ancient lineage induce distinct patterns of immune responses in human macrophages, dendritic cells and whole blood. Pampi Chakraborty et al.
   Infection with different Mycobacterium tuberculosis genotypes in a BALB/c mouse model exhibit differential pattern of cytokine expression, bacterial load and lung pathology. Pampi Chakraborty et al.

c. Papers presented in Conferences:

1) P. Chakraborty, S. Kulkarni, M.G.R. Rajan, K.B. Sainis (2008) To study hostparasite interactions by standardizing infection model using THP-1 cell line and different strains of M.tuberculosis. DAE-BRNS 4th Life Sciences Symposium on Recent Advances in immunomodulation, stress and cancer, Mumbai .
2) S. P. Kulkarni, P. Chakraborty, K. B. Sainis. (2009) The immune subversion of XDR strains of M.tuberculosis isolated from Mumbai. 36th Annual conference of Indian Immunology Society, Bangalore
3) S. Kulkarni, M.Makwana, P. Gupta, P.Chakraborty, M.G.R. Rajan. (2010) Study of polymorphisms in Mycobacterium tuberculosis using TbD1 deletion analysis and spoligotyping. DAE-BRNS Life Science Symposium on Current Trends in Biology and Medicine, Mumbai.
4) P.Chakraborty, S. P. Kulkarni, M.G.R. Rajan, K. B. Sainis. (2011) Study of immune responses in THP-1 cells infected with strains of Mycobacterium tuberculosis from different lineages prevalent in India. Keystone symposium Tuberculosis: Immunology, Cell Biology and Novel Vaccination Strategies. Vancouver, Canada.
5) Pampi Chakraborty, Savita Kulkarni, M. G. R. Rajan, K. B. Sainis. (2011) Differential immune response to different genotypes of M.tuberculosis is a strain dependent phenomenon'. 37th annual conference of Indian Immunology Society, Jammu, February 7-9,.
6) Savita Kulkarni , Sriparna Das, Pampi Chakraborty, M. G. R. Rajan. (2011) Overexpression, purification and immunological characterization of recombinant 38kda antigen of M.tuberculosis. 37th annual conference of Indian Immunology Society, Jammu.
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8) Pramod Kumar Gupta, Pampi Chakraborty, M. G. R. Rajan, Savita Kulkarni.(2012) Modulation of maturation and activation of murine bone marrow derived dendritic cells (BMDCs) by different clinical isolates of M.tuberculosis. U.S.-India Joint Workshop on tuberculosis at International Centre For Genetic Engineering And Biotechnology, New Delhi
9) Sujay Gaikwad, Pampi Chakraborty, Savita Kulkarni, M.G.R Rajan. The lipid profiles of different genotypes of M.tuberculosis and its correlation to in vitro immune response induced by the same stains. 39th Annual Conference of Indian Immunology Society (IMMUNOCON 2012), 9-11 Nov, 2012.Varanasi.
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Title	:	Studies on the Separation and Recovery of Ruthenium

Abstract

The noble metal, ruthenium (Ru) is produced in significant quantity as a fission product in fast breeder reactors and is one of the most troublesome fission products during the reprocessing of spent nuclear fuels as well as the waste management processes due to its large fission yield, relatively long half lives (^{103}Ru: 39.26 days; ^{106}Ru: 373.59 d) and its many oxidation states ranging from 0 to +8. During the dissolution of irradiated nuclear fuel in nitric acid in the PUREX process, various nitrosyl complexes formed by ruthenium show complicated distribution behavior between the aqueous phase and the extract phase and a few of them remain in TBP/Dodecane after stripping; therefore, it is difficult to completely separate ruthenium from uranium and

plutonium which results in the possible release of radio-ruthenium in the environment. During the nuclear waste management processes such as calcination, denitration and vitrification of the high level liquid waste (HLLW), ruthenium undergoes oxidation to form highly volatile radiotoxic RuO_4 which decomposes to non-volatile RuO_2 black solid and deposits over the cooler part of equipment and hence, increases the radiation dose of plant. Hence, it is desirable to separate Ru from HLLW, prior to waste treatment.

Parametric studies were carried out for the separation and recovery of ruthenium from pure nitric acid as well as from simulated high level liquid waste (SHLLW) by chemical and electrochemical volatilization methods. By chemical volatilization method using 0.02-0.04 M ammonium ceric nitrate (ACN) as the oxidizing agent in presence of n-paraffin hydrocarbon, removal of Ru both from pure $RuNO(NO_3)_3$ and SHLLW was quantitative at acidity 0.5 -1M. Separation of Ru from SHLLW was also studied by electrochemical volatilization method using divided/undivided cells, with and without the redox catalyst cerium, by applying constant current/ potential. In the case of undivided cell, quantitative separation of Ru was possible from pure $RuNO(NO_3)_3$ solution prepared in 1M nitric acid in the presence of 0.04 M Ce by applying 20 mA/cm^2 anodic current density, whereas only 50 % of Ru was separated from SHLLW under similar experimental conditions. During the separation of Ru using divided electrolytic cell with glass frit diaphragm, quantitative separation of Ru was possible both from pure $RuNO(NO_3)_3$ solution and SHLLW prepared in 4 M nitric acid by applying 20 mA/cm^2 anodic current density and also without any redox mediator. Separation of Ru was also carried out by applying constant potential using divided cell and near quantitative separation was possible from solutions prepared in 1M nitric acid. As the HLLW is in 4 M nitric acid, the cell configuration with glass frit as the separating membrane is recommended for the separation of Ru in the plant. The redox behavior of $[RuNO]^{3+}$ species in nitric acid medium was investigated by cyclic voltammetry and chronopotentiometry at both Pt and GC working electrodes. A quasi-reversible one electron reduction of $[RuNO]^{3+}$ was observed at both GC and Pt. The diffusion coefficient (D_o) of $[RuNO]^{3+}$ species in the order of 10^{-8} $cm^2.s^{-1}$ was estimated by CV and CP techniques and the heterogeneous electron transfer rate constant (k_s) for reduction of $[RuNO]^{3+}$ in the order of 10^{-5} $cm.s^{-1}$ was estimated using Klingler and Kochi equation using Pt and GC working electrode.

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2. Pravati Swain, S. Annapoorani, R. Srinivasan, C. Mallika, U. Kamachi Mudali, R. Natarajan, Separation of ruthenium from simulated nuclear waste in nitric acid medium using n-Paraffin Hydrocarbon. Separation Science and Technology (2014) 49: 112-120.
3. Pravati Swain, S. Annapoorani, R. Srinivasan, C. Mallika, U. Kamachi Mudali, R. Natarajan, Separation and recovery of ruthenium from nitric acid medium by electro-oxidation. Journal of Radioanalytical and Nuclear Chemistry (Communicated).
4. Pravati Swain, Dr. K. Sankaran, R. Srinivasan, C. Mallika, U. Kamachi Mudali, R. Natarajan, Studies on the Feasibility of Separation of Ruthenium from High Level Liquid Waste by constant potential electro-oxidation. Progress in Nuclear Energy (Under revision)
5. Pravati Swain, C. Mallika, Ch. Jagadeeswara Rao, U. Kamachi Mudali and R. Natarajan, ‘‘Electrochemical studies on the reduction behaviour of [RuNO]3+ in nitric acid medium’’, Journal of Applied Electrochemistry (Communicated).

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4. Pravati Swain, S. Annapoorani, R. Srinivasan, C. Mallika, U. Kamachi Mudali and R. Natarajan, Effect of Ceric Ions in the Extraction of Ruthenium into 30%TBP/NPH Systems. DAE – BRNS Biennial Symposium on Emerging Trends in Separation Science and Technology –SESTEC – 2012, February 27 - March 01, 2012, Mumbai, India. (Best Paper award).
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Abstract

In this thesis work, generation of quasi-monoenergetic electron beams with peak energy about 20 MeV and divergence ^ 10 mrad were demonstrated from laser wakefield acceleration in forward Raman scattering assisted strongly self-modulated regime using sub- mm length helium gas jet plasma as accelerating medium and > 45 fs, < 10 TW laser pulses of intensity > 1x10 W/cm to drive ultrahigh gradient wakefield > 1 0 0 GV/m in the plasma. It was also shown that the self-modulation and consequently electron beam charge and energy could be enhanced up to about 100% and 40% respectively by introducing optimum amount of positive chirp in the laser pulse. Further, the effect of ns duration prepulse pedestal (due to amplified spontaneous emission) on pre-plasma channel formation, intense 45 fs laser pulse propagation and electron acceleration was studied in detail and showed optimum level of pre-pulse for a given gas density forms low density pre-plasma channel suitable for 45 fs laser pulse guiding over few times the natural diffraction length and consequently electron acceleration to higher energy of about 50 MeV. With reduced prepulse level, effect of different gas media (He, N2, and Ar) were investigated and found optimum parameters for producing stable, high quality electron beams with average divergence ~ 10 mrad and central peak energy ~ 35 MeV and 25 MeV from helium and nitrogen gas jets respectively. From Ar gas jet, collimated electron beam of ~ 40 mrad was observed once in a while with energy < 10 MeV. Further, laser wakefield acceleration in laser produced solid plumes was investigated and demonstrated low divergence ~10 mrad, quasi- monoenergetic electron beam with peak energy ~12 MeV from plasma plume produced from solid nylon target. The results are promising for applications of the electron beam with high rep-rate operation of laser wakefield accelerators.

The thesis work also includes study of angular distribution of bremsstrahlung hard x- ray dose due to energetic fast electrons generated from intense laser-solid target plasma interaction. The fast electrons are also characterised under different laser polarization, intensity, and pulse duration irradiation conditions to study angular and energy distribution of the electrons and scaling laws were obtained. These results are useful to understand the physics of fast electron generation and to control the fast electrons for their direct application or to control secondary process like continuous or K_a x-ray generation, ion acceleration, intense magnetic field generation etc.

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3. "Highly collimated quasi-monoenergetic electron beam from laser wakefield acceleration in laser produced plasma plume", B. S. Rao, A. Moorti, P. A. Naik, and P. D. Gupta, Applied Physics Letters 2013, Vol. 102, p. 231108(5 pages).
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10. "Stable high charge electron beam from laser wakefield acceleration using nitrogen gas jet target", B. S. Rao et al., Manuscript under preparation.

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   Received Best Poster Award from the Plasma Society of India
2. "High-quality stable electron beam generation by interaction of 10 TW, 45 fs laser pulses with gas-jet and plasma plume targets", A. Moorti, B. S. Rao, R. Rathore, J. A. Chakera, P. A. Naik, and P. D. Gupta, Laser and Plasma Accelerators Workshop, Goa, India, Sep. 2 - 6, 2013.
3. "Highly-collimated quasi-mono-energetic electron beam by laser wakefield acceleration in laser produced solid target plasma plume", B. S. Rao, A. Moorti, R. Rathore, J. A. Chakera, P. A. Naik, and P. D. Gupta, 4th Asian Forum for Accelerators and Detectors, BINP, Novosibirsk,

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6. "Progress on experimental studies on laser-driven plasma based electron acceleration at RRCAT, India", A. Moorti, B. S. Rao, Chakera J. A. Chakera, P. A. Naik, and P. D. Gupta, International Committee on Ultra-High Intensity Lasers, Mamia, Romania, Sep. 16 - 21, 2012.
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12. "Electron acceleration in self-modulation regime using 10 TW, 45 fs Ti:sapphire laser beam", J. A. Chakera, B. S. Rao, P A. Naik, M. Kumar, and P D. Gupta, International Symposium on Waves, Coherent Structures & Turbulence in Plasmas, IPR, Gandhi Nagar, Jan. 12 - 15, 2010.
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    Received Best Poster Award
17. "Energy spectrum measurement of fast electrons produced in ultra-intense laser solid interaction", B. S. Rao, V. Arora, P. A. Naik, and P. D. Gupta, 22nd National Symposium on

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Title	:	Characterization of HHV-6 using an Indian Isolate : An in in Vitro Study

Abstract

HHV-6B is a double-stranded DNA herpesvirus that is ubiquitous and latent throughout the adult life of most healthy individuals. A HHV-6 positive B-cell line (designated PJH6) was derived from an individual (donor) earlier in the laboratory. Characterization of this isolate in vitro and development of two valuable research tools using the said isolate were undertaken in this study.
The first objective was limited characterizations of the virus isolate including infectivity. Electron microscopy showed characteristic herpesvirus morphological feature and the cell line derived spontaneously generated extracellular virus particles could successfully infect all the target cells as confirmed by HHV-6B specific nested PCR. Further, serial passage of cell free virus particles in SupT1 cells indicated that the isolate was capable of imparting productive infection to host cells.

The second objective was profiling chromosomal integration of the isolate where the site of integration in PJH6 cell line, donor peripheral blood mononuclear cells (PBMC), as well as that of PBMC from father was found to be identical, chromosome 12q14, thus indicating an event of vertical transmission from father to son. This was an atypical integration seen in this cell line as earlier studies of integration reported telomeric regions as preferred sites.

The third objective was to study the role of viral immediate early (IE) gene products on activation of select cellular genes. Though co-transfection experiments using viral IE-1 gene and three target promoters (of c-fos, c-myc and hsp-70 genes) exhibited an increase in their activity by a luciferase assay, infection of SupT1 cell line with the virus showed most significant levels of up-regulation of hsp-70 while c-fos showed marginal up-regulation.

The fourth objective was to develop a HHV-6 genome derived basic vector for gene transfer. Amplicon unit (harboring a GFP expression cassette as the transgene) derived pseudovirions were used to transduce various cell lines including HEK293, Daoy, SupTI, and U937. GFP transgene expression was retained at high levels after antibiotic selection of the transduced HEK293 cells thus validating the functionality and stability of the amplicon vector.

The fifth objective was to develop a luciferase reporter based single step relative viral titer estimation assay for HHV-6 by developing an indicator HEK293 cell line. Using cell free virus preparations the reporter gene expression from the indicator cells showed a positive correlation with serial viral dilutions validating the assay.

The reported thesis thus made basic characterization of the only Indian HHV-6 isolate along with development of two valuable tools, i.e., a gene transfer vector and a virus titer assay, which will be helpful for further studies on HHV-6 biology.

Publications

Pallavi Goel, Prafullakumar Tailor, Ajit G. Chande, Atanu Basu, Robin Mukhopadhyaya,. An infectious HHV-6B isolate from a healthy adult with chromosomally integrated virus and a reporter based relative viral titer assay.

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Title	:	Spectroscopic Investigations on the Properties of Two Drugs: Curcumin and Chlorin p6

Abstract

In this thesis the properties of two drugs, Curcumin and Chlorin p_6 (Cp6) in different environments were studied by different spectroscopic techniques. The photophysical properties of Curcumin in various toluene-polar solvent mixtures using time resolved fluorescence spectroscopic technique. The results obtained shows that excited state hydrogen transfer (ESHT) reactions in the excited state of Curcumin depend critically upon the hydrogen bonding property of the polar solvent. The rate limiting step in the ESHT process of Curcumin in these solvent mixtures might be the formation and reorganization of the intermolecular H-bonding between the keto group of the pigment and the hydrogen bond donating property of the polar solvent. The diffusion characteristics of Cp6 and two other dyes are studied using the interfacial second harmonic (SH) generation spectroscopic technique. The diffusion of Cp6 across a liposome can be measured at acidic pH (3-5). Further, at this pH range, increasing the bilayer rigidity significantly affects the diffusion characteristics of the drug. The aspects of drug induced membrane permeability were studied using the two drugs Curcumin and Cp6. It has been observed that the diffusion kinetics of two organic cations depends significantly upon the nature of the drug as well as the pH of the medium.

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across a negatively charged lipid bilayer probed by second harmonic spectroscopy", R. K. Saini, G. K. Varshney, A. Dube, P. K. Gupta, K. Das. (Under revision)

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Title	:	Evaluation of Structure-Function Relationship of Photosynthetic Machinery in Cyanobacteria Exposed to Chromium (VI) Stress

Abstract

Cyanobacteria were the first organisms to generate oxygen during photosynthesis.They originated ca. 3.5 billion years ago in the course of evolution of life and have evolved elaborate mechanisms to resist several environmental stresses, metal stress being one of the important stresses. All metals are toxic beyond a certain concentration. In natural habitats, aquatic micro-flora may be chronically exposed to various toxic metals. Among the toxic metals, chromium (Cr) is a major concern for aquatic photoautotrophs. Cr (VI) is highly mobile and hence available, resulting in biological toxicity mainly due to oxidative damage to bio-molecules. Microorganisms, including photoautotrophs, in the contaminated sites have evolved various mechanisms and metabolic adjustments for chromate tolerance. Adaptive changes brought about in photosynthesis in the chromate resistant photoautotrophs by chronic exposure to Cr (VI) have not been studied.

In the thesis, entitled “Evaluation of Structure-Function Relationship of Photosynthetic Machinery in Cyanobacteria Exposed to Chromium (VI) Stress“ two unicellular, non-nitrogen fixing cyanobacteria, Synechococcus elongatus PCC7942 and Synechocystis sp. PCC 6803 were examined for their tolerance to Cr (VI). Synechococcus showed 12 times higher tolerance as compared to Synechocystis with EC_{50} of 150 + 15gM and 12 + 2gM, respectively. Interestingly, Synechococcus showed stimulation of growth at concentrations of chromate less than 100gM, which affected its cell size without disturbing ultra-structure and thylakoid organization. In Synechocystis, growth with 12gM potassium dichromate damaged the ultra-structure and thylakoid organization. Using labeled chromate, slight accumulation (< one nanomole/10^8cells) was observed in Synechocystis; no accumulation of chromate could be observed in Synechococcus. IC50 values of chromate for sulfate uptake were higher in Synechococcus as compared to Synechocystis. The results suggested that the sulfate transporters in Synechococcus have lower affinity to chromate than those from Synechocystis indicating differences in affinity of sulfate receptors for chromate in the two organisms. Therefore, lesser uptake of chromate may be one of the reasons for tolerance to Cr (VI) in case of Synechococcus. Cr (VI) is known to manifest its toxicity by causing oxidative stress. At lower concentrations, Cr (VI) caused excessive ROS generation in Synechocystis as compared to that observed in Synechococcus. Intrinsic levels of enzymatic antioxidants i.e. catalase and 2-Cys-Peroxiredoxin were considerably higher in Synechococcus than Synechocystis. This correlated well with higher content of carbonylated proteins observed in Synechocystis than Synechococcus. The data suggested that inherent activity/content of antioxidant enzymes may also have an important role in determining tolerance of these cyanobacteria to Cr (VI).

As cell membranes and photosynthetic apparatus are known to be the targets of Cr (VI), effect of Cr (VI) on photosynthetic machinery in the cyanobacteria was studied. Growth with dichromate reduced chlorophyll, phycocyanin and carotenoid contents in both the cyanobacteria without affecting their spectral quality. It also reduced the rate of CO_2 fixation, PSII and PSI activities and PSII/PSI ratio in addition to F_v/F_m as well as P_m in both the cyanobacteria. However, effective quantum yield of PSII and PSI increased on growth with dichromate in Synechococcus whereas it decreased in Synechocystis. The quantum yield of cyclic electron flow increased in both the cyanobacteria on growth with Cr (VI). Thus in addition to intrinsic difference in photosynthetic rate, the two cyanobacteria also showed differential modulation of photosynthetic machinery in response to chronic Cr (VI) stress. The responses of the cyanobacteria exposed to Cr (VI) to other oxidative stresses like high-intensity light and H2O2 were interesting. The photosynthetic

machinery of Synechocystis exhibited better tolerance to the oxidative stresses after being exposed to Cr (VI) as compared to Synechococcus. These results suggested that Cr (VI) stress brings about adaptive modifications in Synechocystis which enable it to tolerate extra oxidative stresses.

The first step of photosynthesis has inspired a major field of research of artificial photosynthesis. As Synechococcus was able to maintain its major photosynthetic functions at relatively higher dichromate concentrations by making adjustments in the photosynthetic apparatus, the antenna functionality of its light harvesting pigments was studied for potential use as a sensitizer in dye sensitized solar cells. Pigments of the antenna complex from control and chromate grown cells of Synechococcus were isolated and analyzed for their suitability for energy capture and transfer in the artificial system.

Thus, the comparative study on chromate tolerance in these two cyanobacteria showed differential response and novel mechanisms of adaptation to excessive chromate in media.

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Title	:	Modeling and Measurement of Radon and Thoron Emission from Naturally Occurring Radioactive Materials

Abstract

Radon is a natural radioactive gas that occurs ubiquitously in the environment. There are three natural isotopes of radon namely ^{222}Rn (radon), ^{220}Rn (thoron), and ^{219}Rn (actinon) formed from the alpha decay of radium as a part of the decay series of ^{238}U (uranium), ^{232}Th (thorium), and ^{235}U (actinium), respectively. Based on the results of case-control studies in Europe & North America, the World Health Organization indicated that exposure due to ^{222}Rn, ^{220}Rn and their decay products in environment could be the second most important cause of lung cancer, next to smoking. These findings and inference have led to a renewed interest in the subject of radon studies. The quantification of the radon source terms in the environment requires accurate techniques for the measurement of emission rates from various Naturally Occurring Radioactive Materials (NORMs) such as soil, building materials etc. The most commonly used techniques, which are also simple and convenient for large scale deployment, are based on measuring the build-up of radon in soil chambers for the case of emissions from soil and closed cans for the case of building materials. Through a careful study of literature, it was found that there exist several shortcomings in the models used for the analysis of the response of systems. To overcome these

shortcomings, this thesis primarily addresses the development of process based models, analysis of their implications and experimental validations for the $^{222}Rn/^{220}Rn$ emission measurement techniques, both for outdoor and indoor environment. A two dimensional, two-region, diffusion process based, Non Steady State (NSS) model is developed and solved analytically to quantify the response of the soil chamber deployed on soil surface. The 2-D model enables a simple surface chamber deployment protocol as compared to the deep insertion protocol, commonly used to meet the assumptions of the case of 1-D model. Another important aspect of the 2-D model is that it provides simultaneous information of pre-deployment emission flux and soil diffusion coefficient. The model predicts an instantaneous flux drop due to change in the gas mixing process during deployment of the chamber. The model also predicts other parameters such as saturating concentration in the chamber and its time response, useful parameters for selecting appropriate size of chamber for different applications in environmental specific studies. Experimental validation of the 2-D model has been carried out by conducting systematic experiments at a uranium mineralized zone, Jaduguda. Subsequent to its validation, practical applicability of the 2-D model is demonstrated by studying flux profile across a sealed surface, a mixed boundary value problem. A good matching has been observed between chamber based measurement and diffusion theory based flux estimate. To correctly predict the indoor emission source term due to walls, a semi-empirical model is proposed which requires input parameters such as emission rate of building materials samples, radon diffusion length in the materials, dimension of the samples and thickness of the wall. Study indicated that there exists a large difference in the surface emission fluxes from building materials samples and that from a wall made by these materials. This fact was also supported by experimental results. It is hoped that the various developments presented in the thesis will go a long way in strengthening our confidence in the assessment methods, so as to provide a realistic perspective of the radon, thoron issues in the country and elsewhere in the world.

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Title	:	Development of SQUID Based Magnetocardiography System & Cardiac Signal-Source Analysis using Ensemble Empirical Mode Decomposition

Abstract

MagnetoCardioGraphy (MCG), which is the magnetic counterpart of the surface ElectroCardioGraphy (ECG), measures the magnetic field (typically 50pT at QRS peak) produced by the electrical activity of the myocardial tissues constituting the heart in a non-invasive and non-contact way by harnessing the highly sensitive Superconducting QUantum Interference Devices (SQUIDs). The inherent advantages of the MCG technique have been explored in clinical research over the last two decades and is now receiving considerable attention. In view of this, several research groups, including that at IGCAR, Kalpakkam, have established multichannel MCG systems. These enable simultaneous measurements of magnetic fields at a discrete set of points on the thorax to generate a comprehensive picture of the magnetic field distribution, which makes it possible to visualize the cardiac source in terms of current density maps and source reconstruction through the solution of the inverse problem.

This thesis describes the efforts involved in the assembly and wiring of a multichannel MCG measurement facility and in using the facility to record multichannel MCG data. Since the measured MCG data often has a low signal-to-noise ratio (SNR), it was essential to explore methods to denoise the measured data prior to using for estimation of source parameters. Towards this, Ensemble Empirical Mode Decomposition (EEMD) based approach was developed and its performance in enhancing the SNR was assessed by comparing it with other standard denoising techniques based on wavelet transform and Independent Component Analysis (ICA). A combination of EEMD and ICA applied to the multichannel MCG data is shown to have the twin advantages of significant improvement in SNR and a lower computational burden. An assessment of the performance of the combination of EEMD and ICA has been compared with other standard techniques such as the use of ICA alone and wavelet enhanced ICA (wICA). The denoised data has been used for the construction of pseudocurrent density maps and for estimation of source parameters in the context of a single equivalent current dipole model. The effect of signal denoising on the pseudocurrent density maps and on the estimation of source parameters is discussed.

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Title	:	Energy Transport in Inertial Confinement Fuision Plasmas

Abstract

Inertial Confinement Fusion (ICF) is an approach to attain controlled nuclear fusion by using high power lasers or charged particle beams as drivers to create high energy density plasma. Plasma heating by charged particles and neutrons, energy exchange between ions and electrons and radiation losses are the primary mechanisms determining the ignition conditions in a thermonuclear plasma. In this thesis, we analyze the effects of elastic nuclear scattering, large angle Coulomb scattering and collective plasma effects on the thermalization distance and energy leakage probability of the charged fusion products in a deuterium (D) and deuterium-tritium (DT) plasma. We also develop a simple model for energy deposition by the neutrons as a result of nuclear interaction with the ions. This improved energy deposition scheme is applied to a zero-dimensional model which solves the rate equations for the ions and three temperature (3T) energy equations for ions, electrons and radiation. The concept of internal T breeding is reevaluated using this model and it is found that tritium breeding improves significantly in comparison with earlier estimates. We obtain optimum parameters for the initial pellet temperature, density and T fraction for which T acts as a catalyst, helps in reducing the ignition temperature and the D in the pellet burns sufficiently before the pellet disassembles. Modifications have been made in the model to include central ignition and yields have been obtained for DT pellets having a wide range of initial densities and temperatures.

Radiation transport and its interaction with matter via emission, absorption and scattering of radiation have a substantial effect on both the state and motion of materials in high temperature

hydrodynamic flows occurring in high energy density systems. Non-equilibrium radiation transport equation is non-linearly coupled to the material energy equations with the material properties having complex dependence on the independent variables. Time dependent radiation transport codes are commonly solved numerically. Nevertheless, analytical benchmark results for test problems are necessary to validate and verify the numerical codes. In this thesis, new analytical benchmark solutions have been obtained for a finite planar slab, sphere and spherical shell using both the Laplace transform and eigenfunction expansion method. 1D codes are also developed for hydrodynamics, radiation diffusion and transport simulation. Finally, a fully implicit 1D radiation hydrodynamics code is developed by coupling implicit finite difference hydrodynamics with time dependent radiation transport. The results agree with the scaling law for radiation driven strong shock propagation through Al in the planar geometry and point explosion with heat conduction in the spherical geometry. Having, thus, benchmarked the code, self convergence of the method w.r.t., time step is studied in detail for both the planar and spherical problems. Spatial as well as temporal convergence rates are ~ 1 as expected from the difference forms of mass, momentum and energy conservation equations. At the initial stages of ICF implosion, when phase transition from the solid to liquid phase occurs, accurate knowledge of the melting point for various pressures is essential for choosing the proper EOS to be used for hydrodynamic simulation. The melting curves of Cu and Al have been obtained using classical molecular dynamics simulation. Role of random and site-selective substitution of Ti in Cu is also analyzed in terms of the Radial Distribution Function (RDF).

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Title	:	Effect of Sinter Additives on the Consolidation and Properties of Titanium Diboride Composites

Abstract

Consolidation of TiB_2 is a challenge due to its high melting point; covalent nature requires high temperatures for sintering. However, borides undergo an abnormal grain growth at high temperatures. The occurrence of microcracking at the grain boundaries is also promoted with the increase in grain size. Thus, it is very difficult to achieve crack free dense borides by the conventional cold compaction and sintering, as no shape accommodation occurs without an external pressure and large pores tend to coarsen during high temperature sintering.

In order to overcome the above issues it is very essential to add a suitable sinter additive. Choice of sinter additive is a challenge to obtain a density without losing its (TiB_2) inherent properties. Silicides have attracted considerable interest due to their compatibility with borides to densify at lower temperatures. In the present investigations, various silicides were used to densify the TiB_2 by hot pressing. Silicides not only lowered the densification temperature, but also helped to improve the toughness and oxidation resistance. Reactive sintering and liquid phase sintering were the main densification mechanism in all the cases. Silicon in the silicides helped to reduce the surface oxides of TiB_2, which is advantageous as mentioned above. Presence of reaction product/secondary phase helped to improve the fracture toughness by crack deflection or bridging mechanisms. However, presence of silicon also helped to improve the oxidation resistance by formation of a thin glassy layer on the surface. Effect of various silicides and its quantity on the densification, properties and oxidation behavior was mainly studied in this thesis.

Publications

International Journal Publications out of this thesis

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Title	:	Methodology and Estimation of Software Reliability for Safety Systems

Abstract

Software design, development and testing have become very intricate with the advent of modern highly distributed systems, networks, middleware and interdependent applications. In nuclear power plants (NPP) many systems are being used in Safety Critical and Safety Related applications, which demand a very high reliability. As software becomes an increasingly important part of many different types of systems that perform complex and critical functions in many applications, such as defense, nuclear reactors, etc., the risk and impacts of software caused failures have increased. There is now a general agreement on the need to increase software reliability by eliminating errors made during software development.

Software is designed to perform a set of specified functions. Upon execution of a program, an input state is translated into an output state. An input state can be defined as a combination of input variables or a typical transaction to the program. When the actual output deviates from the expected output, a failure occurs. Software faults are most often caused by design faults. Design faults occur when a designer, misunderstands a specification or makes a mistake. Software reliability is defined as the probability of failure-free software operations in a specified environment.

The main objective of the research is the estimation of software reliability for safety systems of NPP. In the process of assessment of reliability the following sub-objectives are envisaged since software reliability is more concerned with design, methodologies, practices and the tools used in the process of software development. The sub-objectives are
(a) Development of software life cycle model for safety critical systems.
(b) Determination of software metrics & development of software metric tool.
(c) Development of Software Verification and Validation methodology.
(d) Development of Software Reliability Model.
(e) Estimation of Software Reliability for Safety systems of NPP

The Research work is specifically for the software development on Instrumentation & Control systems employed in NPP. The reliability estimation is based on the following parameters: Cyclomatic Complexity, Local & Global Variables, Nesting Levels, Kilo Lines of code, Adherence to the standards, V&V iterations, Number of functions, Comment to code ratio and Number of interrupts. Robustness and validation of the methodology has been demonstrated by applying it to software deployed in Safety Critical & Safety Related systems of a Fast Reactor.

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Title	:	Mössbauer Investigations on Fe Based Nano Spinel Ferrites

Abstract

Cubic iron oxide nanoparticles such as magnetite find a wide ranging applications spanning from high density magnetic memory devices, magnetically guided drug delivery, hyperthermia to spintronic devices. Understanding of the Verwey transition (high temperature metallic to insulating) in this system at 120 K still remains incomplete. The thesis mainly addresses some of the important issues related to local structure and magnetic properties of the nanoparticles of magnetite using a detailed ^{57}Fe based Mossbauer spectroscopy.

Evolution of nanoparticles of off-stoichiometric magnetite and goethite formed in the co precipitation process to stoichiometric magnetite due to controlled annealing treatment has been studied in a detailed manner. Stability of magnetite nanoparticles capped with oleic acid surfactant and bound in zeolite template based on the hyperfine parameters and their systematic variations with annealing treatments. A strong binding of oleic acid by off stoichiometric magnetite and goethite nanoparticles has been exploited to obtain stoichiometric nanoparticles of magnetite limiting the size of these particles to less than 12 nm and a detailed Mossbauer studies have been carried out at different temperatures between 300 – 80 K.

Point defects aspects in off stoichiometric nanoparticles of magnetite have been studied in a detailed manner to understand the cationic occupation. Also the role of point defects in inducing ferromagnetism in zinc ferrite nanoparticles is elucidated based on the systematics of the Mossbauer results obtained due to the coarsening of the particles. These results are compared with that of bulk zinc ferrite subjected to vacuum ($\approx 10^{-6}$ mbar) annealing at elevated temperature.

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4. “Point defects aspect of magnetite nano particles as studied by Mossbauer spectroscopy”, L

Herojit Singh, R Govindaraj, G Amarendra and C. S. Sundar, AIP Conf Proc, 1447, 445 (2012)

5. "Partial inversion in nano zinc ferrite as studied using Mossbauer spectroscopy", L Herojit Singh, R Govindaraj, G Amarendra and C. S. Sundar, AIP Conf. Proc., 1512, 322 (2013)
6. "Mossbauer Studies of Local Environments of 57Fe in Iron Oxide Particles Dispersed Fe Matrix", L. Herojit Singh, R Govindaraj, P. A. Kumar, G. Amarendra, C. S. Sundar, AIP Conf. Proc., 1349, 423 (2011)
7. "Studies on local structure and magnetic properties of polymorphs of iron oxides by Mossbauer spectroscopy", L. Herojit Singh, R. Govindaraj, G. Amarendra and C. S. Sundar, MRSI 2010, Trivandrum
8. Defect induced ferromagnetism and recovery in $ZnFe_2O_4$, (Manuscript under preparation)
9. Linear correlation between hyperfine parameters as observed in the thermal evolution of iron oxide nano particles, (Manuscript under preparation)
10. Aspect of local structure and magnetic properties in chemically synthesized magnetic nanoparticles as studied using Mossbauer spectroscopy, (Manuscript under preparation)

List of publications and conference proceedings not pertaining to thesis work:

1. "Annealing effects in Eurofer-97 steel as studied by Mossbauer spectroscopy", L. Herojit Singh, S. Hari Babu, R. Govindaraj, G. Amarendra, and C. S. Sundar, AIP Conf. Proc, 1447, 1321 (2012)
2. "Mossbauer Spectroscopic studies in Ni-Fe-Co Alloy", L. Herojit Singh, R. Govindaraj, C. Ravishankar, G. Amarendra and C. S. Sundar, MRSI-AGM, (2013)

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Abstract

Some aspects of the interplay between bipartite correlations and quantum channels", Krishna Kumar Sabapathy.

This thesis explores ways in which quantum channels and correlations (of both classical and quantum types) manifest themselves, and also studies the interplay between these two aspects in various physical settings. Quantum channels represent all possible evolutions of states, including measurements, allowed by quantum mechanics, while correlations are intrinsic (nonlocal) properties of composite systems. There are four main problems that was addressed in each of the main Chapters in the thesis: (i) The role played by initial system-bath correlations on the subsystem dynamics of an open quantum system. Only product initial system-bath states lead to completely positive system dynamics, disproving a recent claim in literature.

(ii) Computation of correlations for two-qubit X-states, namely, classical correlation, quantum discord, and mutual information: the optimal measurement is obtained by finding the root of a single variable function. The method exploits the complete geometric nature of the problem and clarifies and corrects many results recently published by a few authors.

(iii) The robustness of non-Gaussian entanglement under symmetric local noisy attenuator and amplifier channels: we demonstrate simple examples of nonGaussian states with 1 ebit entanglement that are more robust that all Gaussian states with arbitrary large entanglement.

(iv) Connection between nonclassicality breaking and entanglement breaking for single-mode bosonic Gaussian channels: we introduce the notion of nonclassicality breaking channels are

bring out the differences and similarities with respect to the well-known notion of entanglement breaking channels.

Publications

1) Robustness of nonGaussian entanglement against noisy amplifier and attenuator environments. K. K. Sabapathy, J. S. Ivan, and R. Simon. Physical Review Letters, 107, 130501 (2011).
2) J. S. Ivan, K. K. Sabapathy, and R. Simon. Operator-sum Representation for Bosonic Gaussian Channels. Physical Review A, 84, 042311 (2011);
3) Nonclassicality breaking is the same as entanglement breaking for bosonic Gaussian channels. J. S. Ivan, K. K. Sabapathy, and R. Simon. Phys. Rev. A, 88, 032302 (2013).
4) Quantum discord for two-qubit X-states: A comprehensive approach inspired by classical polarization optics. K. K. Sabapathy and R. Simon. arXiv:1311.0210 [quant-ph].Quantum discord plays no distinguished role in characterization of complete positivity: Robustness of the traditional scheme. K. K. Sabapathy, J. S. Ivan, S. Ghosh, and R. Simon. arXiv:1304.4857 [quant-ph].

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Title	:	Extraction and Separation Studies of Uranium and Thorium from Various Aqueous Media using Organophosphorous Extractants

Abstract

2-ethyl hexyl phosphonic acid 2-ethyl hexyl mono ester (PC88A) and di-nonyl phenyl phosphoric acid (DNPPA) are the close analog of di-2-ethyl hexyl phosphoric acid (D2EHPA). Extraction of metal ions using these extractants occurs mostly via cation exchange mechanism. Our literature survey shows that no detailed study has been done on extraction behavior of U(VI) from nitric acid medium using PC88A as well as DNPPA as extractants. Therefore, the aim of the present thesis is to investigate the extraction behavior of U(VI) from HNO_3 medium using these extractants to establish the exteaction mechanism and the evaluation of the effects of various parameters such as diluents, extractant and metal ion concentration, temperature and stripping agents. The presence of neutral donors such as TBP, TOPO, MIBK (methyl isobutyl ketone), DOSO (di octyl sulphoxide), Cyanex 923 showed synergism. Synergistic coefficients (S.C) at different nitric acid concentrations were calculated and correlated with their acid uptake constants. An attempt has been made to develop empirical model for the U(VI) extraction from H_2SO_4 medium using PC88A and its mixture with neutral donors like TOPO in n-dodecane. Further studies were carried out for process development for separation of U(VI)-Th(IV) from monazite leach solution using novel solvent tris-2-ethyl hexyl phosphate (TEHP). Uranyl nitrate raffinate (UNR) waste generated from uranium purification plant is an important secondary source of uranium which contains <1 g/L uranium and a large number of other metal ions as impurities. In this thesis an attempt has been made for Supported Liquid Membrane (SLM) treatment to recover high purity uranium from this raffinate. Different organophosphorous extractants such as (a) acidic (HA): PC88A, Cyanex 272, DNPPA, D2EHPA; (b) neutral (S): TBP, TEHP, TOPO, TEBP, Cyanex 923 and their different synergistic combination dissolved in n-paraffin were used as carriers impregnated in polytetrafluoroethylene (PTFE) membrane. Investigation have also been carried out on the aggregation behavior of DNPPA under varying experimental conditions such as aqueous phase acidity, nature of diluents, and ligand concentration using Dynamic Light Scattering (DLS), spectrophotometry. The aggregation behavior has been correlated with the extraction properties of metal ions such as U(VI) from HNO_3 medium. A simple spectrophotometric technique is described in this thesis for the determination of uranium in ore leach solutions. The technique is

based on the selective extraction of uranium from multi-elemental system using a synergistic mixture of PC88A + TOPO in cyclohexane and simultaneous color development in organic phase using 2-(5-bromo-2-pyridylozo)-5-diethyl aminophenol (Br-PADAP) as chromogenic reagent.

Publications

Journals

1. Synergistic extraction of uranium with Mixtures of PC88A and neutral donors, S.Biswas, P.N.Pathak, D.K.Singh, S.B.Roy, V.K.Manchanda, J. Radioanal. Nucl.Chem. 284 (2010) 13-19.
2. Mathematical modeling of solvent extraction of uranium from sulphate media employing 2-ethylhexyl phosphonic acid-mono-2-ethylhexyl ester (PC88A) and its mixture with tri octyl phosphine oxide (TOPO) as extractants, S. Biswas, P.N. Pathak, D.K. Singh, S.B. Roy, V.K. Manchanda, J. Radioanal. Nucl.Chem. 289 (2011) 557-564.
3. Evaluation of dinonyl phenyl phosphoric acid (DNPPA) and its synergistic mixtures with neutral oxodonors for extraction and recovery of uranium from nitric acid medium, S. Biswas, P.N. Pathak, D.K. Singh, S.B. Roy, V.K. Manchanda, Int.J.Miner.Process., 104-105 (2011) 17-23.
4. Evaluation of 2-Ethylhexyl Phosphonic Acid Mono 2-Ethylhexyl Ester (PC88A) and its Synergistic Mixtures for Uranium Transport Studies from Nitric Acid Medium, Sujoy Biswas, P.N. Pathak, S.B. Roy and V.K. Manchanda , Sep. Sci. Technol. 46 (2011) 592-600.
5. Uranium permeation from nitric acid medium across supported liquid membrane impregnated with acidic organophosphorous extractants and their synergistic mixtures with neutral oxodonors, Sujoy Biswas, P.N. Pathak, Sangita Pal, S.B. Roy, P.K.Tewari and V.K. Manchanda, Sep. Sci. Technol. 46 (2011) 2110-2118.
6. Effect of Alkyl Substituents of Organophosphorous Extractants on Uranium Permeation for Recovery from Uranyl Nitrate Raffinate, Sujoy Biswas, P.N. Pathak, S.B. Roy and V.K. Manchanda, Des. Water. Treat., 38 (2012) 151–158.
7. Carrier facilitated transport of uranium across supported liquid membrane using dinonyl phenyl phosphoric acid and its mixture with neutral donors, S.Biswas, P.N.Pathak, S.B.Roy, Desalination 290 (2012) 74–82.
8. Development of an extractive spectrophotometric method for estimation of uranium in ore leach solutions using 2-ethylhexyl phosphonic acid-mono-2-ethylhexyl ester (PC88A) and tri-n-octyl phosphine oxide (TOPO) mixture as extractant and 2-(5-bromo-2-pyridylozo)-5-diethyl aminophenol (Br-PADAP) as chromophore, S.Biswas, P.N.Pathak, S.B.Roy, Spectrochimica Acta Part A 91 (2012) 222– 227.
9. Kinetic Modeling of Uranium Permeation Across a Supported Liquid Membrane Employing Dinonyl phenyl phosphoric acid (DNPPA) as the Carrier, Sujoy Biswas, P.N. Pathak, S.B. Roy, Int. J. Ind. Eng. Chem. 19 (2013) 547–553.
10. An insight into the speciation and extraction behavior of Eu(III) with dinonyl phenyl phosphoric acid and di(2-ethylhexyl) phosphoric acid: Solvent extraction and fluorescence Studies, Sujoy Biswas, P.N. Pathak, S.V. Godbole, S.B. Roy, Sep. Sci. Technol, 48: 2418–2424, 2013.

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Title	:	Conducting Polymer Field Effect Transistors and Gas Sensors

Abstract

A novel interfacial polymerization at liquid/air interface has been used for the synthesis of freestanding polypyrrole films. In this method a solution consisting of 1mM porphyrin-derivative (TPPOH) and 0.01-1M pyrrole is dropped onto 0.1M aqueous $FeCl_3$ solution kept in a beaker. TPPOH/PPy bilayer forms spontaneously at the air/$FeCl_3$ interface, which after washing in dichloromethane yielded in free-standing PPy nanosheets. Detailed investigation revealed that TPPOH quickly forms J-aggregate films at air/FeCl3 interface, which acts as an in-situ template for the growth of PPy nanosheets. These nanosheets are typically 100-150 nm thick. The room temperature conductivity of polypyrrole sheets synthesized without and with TPPOH template were respectively, 5*10'^{6} and 3x10'^{5} Scm"^{1}. The charge carrier mobility (p) at 300K was found to be 5.34x10"^{5} $m^2V'^1s"^1$. The low temperature resistivity measurements indicated that charge transport occurs via variable range hopping conduction (VRH). Polypyrrole nanosheets exhibited an enhanced response towards NH_3 with typical response and recovery times (for 50 ppm) of 240 s and 50 min, respectively.

We have fabricated first ever field effect transistors in top contact top gate geometry were fabricated using freestanding polypyrrole nanosheets as an active channel. The on-off ratio of the device was found to be ~20. However, there are still some issues pertaining to the mechanical strength of the device, which need to be improved.

Freestanding polypyrrole films were also synthesized using another innovative method at air/liquid interface via acidic oxidation of terpyrrole. The conductivity of these polypyrrole films is found to be ~10^{-7} Scm^{-1}.The hysteretic current-voltage characteristics were gainfully used for demonstration of resistive memory devices.

The flexible polypyrrole-silver nanocomposite films have been prepared on N-(3-trimethoxysilylpropyl)pyrrole modified biaxially oriented polyethylene terephthalate (BOPET) substrate by photopolymerisation of pyrrole using $AgNO_3$ as a photo-initiator.

These nanocomposite films are well adherent, flexible and mechanical very strong. The room temperature electrical conductivity of these films is ~15 Scm^{-1}, which is attributed to the high conjugation length, incorporation of Ag nanoparticles and ordered structure due to the template effect of the silanised pyrrole layer. The polypyrrole-silver nanocomposite films show a reversible conductivity change in the opposite manner on exposure to ppm levels of H_2S and NH_3 gases. A mechanism has been proposed to explain these antagonistic responses for reducing gases.

We have demonstrated fabrication of flexible field-effect transistors (FETs) using poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)], PCDTBT, as an active channel, poly(methyl methacrylate) (PMMA) as gate dielectric and biaxially oriented polyethyleneterephthalate (BOPET) as supporting substrate.The devices exhibit on-off ratio of ~10^5 and mobility of ~10^{-4} $cm^2V'^1s'^1$, which can be further improved. These devices were highly stable under atmospheric conditions (temperature: 20-35°C and relative humidity: 70-85%), as no change in mobility was observed on a continuous exposure for 70 days. The studies on the effect of strain on mobility revealed that devices are stable up to a compressive or tensile strain of 1.2%, indicating that PCDTBT is a very promising active layer for the air stable and flexible FETs.

Publications

[1] P. Jha, S. P. Koiry, V. Saxena, P. Veerender, A. K. Chauhan, D. K. Aswal, S. K. Gupta, Growth of free-Standing polypyrrole nanosheets at air/liquid interface using J- aggregate of porphyrin derivative as in-situ template, Macromolecules. 44 (2011) 4583-4585.

[2] Purushottam Jha, Niranjan S. Ramgir, Preetam K. Sharma, N. Datta, S. Kailasaganapathi, M. Kaur, S. P. Koiry, V. Saxena, A. K. Chauhan, A. K. Debnath, Ajay Singh, D. K. Aswal, S. K. Gupta, Charge transport and ammonia sensing properties of flexible polypyrrole nanosheets grown at air-liquid interface, Materials Chemistry and Physics, 40 (2013) 300-306.

[3] Purushottam Jha, Shankar P. Koiry, Vibha Saxena, Putta Veerender, Abhay Gusain, Anil K. Chauhan, Dinesh K. Aswal, Shiv K. Gupta, Incorporation of non-conjugated polymer chain in conjugated polymer matrix: A new single step strategy for free standing non-volatile polymer memory, Organic Electronics, 14 (2013) 2896-2901.

[4] Ajay Singh, Zakaria Salmi, Nirav Joshi, Purushottam Jha, Ashwini Kumar, Helene Lecoq, Stephanie Lau, Mohamed M Chehimi, Dinesh K. Aswal, Shiv K. Gupta, Photo- induced synthesis of polypyrrole-silver nanocomposite films on N-(3- trimethoxysilylpropyl) pyrrole-modified biaxially oriented polyethylene terephthalate flexible substrates, RSC Advances, 3 (2013) 5506-5523.

[5] P. Jha, S.P. Koiry, Vibha Saxena, P. Veerender, Abhay Gusain, A. K. Chauhan, A. K. Debnath, D. K. Aswal, S. K. Gupta, Air-stability and bending properties of flexible organic field-effect transistors based on poly[N-9'-heptadecanyl-2,7-carbazole-alt- 5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)], Organic Electronics, 14 (2013) 2635-2644.

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Title : Software Reliability in Safety Critical Supervision and Control of Nuclear Reactors

Abstract

1. Context

Software based systems have several advantages over hardware based systems in terms of functionality, cost, flexibility, maintainability, reusability, etc. However, software is prone to failure. Poorly written safety-critical software may lead to catastrophic failures and life threatening situations. Hence, safety-critical software must be adequately tested; and the probability of occurrence of software failures must be studied.

Quantification of software reliability is considered an unresolved issue; and existing approaches and models have assumptions and limitations which are not acceptable for safety applications. Also, to build reliable software, it is necessary to study the factors which are likely to affect the software reliability.

2. Objectives

1. To propose an automated method to generate test cases, and to determine test adequacy in safety-critical software.
2. To propose an approach to quantify software reliability in safety-critical systems of nuclear reactors.
3. To study the factors affecting software reliability in such safety systems.
4. To understand the relationship between the software reliability and number of faults remaining in the software.

5. To understand the relationship between the software reliability and safety in safety critical systems.

3. Method

To quantify the software reliability, a hybrid approach using software verification and mutation testing is proposed. Techniques to solve related issues such as quantification of software test adequacy and detection of equivalent mutants are also presented. The steps proposed to quantify software reliability are:

1. Generation of large number of test cases, where each test case has a unique execution path. To achieve this, code coverage information and genetic algorithms are used.
2. Verification of test cases using a semi-formal model, which is traceable to requirements; and acts as a test oracle.
3. Calculation of test adequacy for the above generated test cases in the range [0,1] using mutation score and conservative test coverage.
4. Calculation of software reliability using the computed test adequacy and the amount of verification carried out.

The formulae for software reliability are derived, and the factors affecting software reliability are presented. The proposed methods are applied to software in the following instrumentation and control systems for fast breeder reactors:

1. Fresh Sub-assembly Handling System (FSHS)
2. Reactor Startup system (RSU)
3. Steam Generator Tube Leak Detection system (SGTLD)
4. Core Temperature Monitoring System (CTMS)
5. Radioactive Gaseous Effluent System (GES)
6. Safety Grade Decay Heat Removal system (SGDHR)

Also, for each case study, mutant characteristics during mutation testing, and the relationship between software reliability and safety are presented.

4. Major results

1. For the case studies, the proposed test case generation technique has resulted in high test adequacy. Using the generated test cases, the probability of software failure in the case studies has been demonstrated to be $< 10^{-5}$ for a random input from the input domain, with 95% confidence level.
2. In mutation testing, for an effective set of test cases, the unkilled mutants have been found to have lower variance in their properties when compared to the killed mutants.
3. Three factors: (i) test adequacy, (ii) the amount of verification carried out, and (iii) the amount of verified code reused; have been found to be affecting the software reliability.
4. The results of present study suggest that software reliability estimates based on the number of faults present in the software alone, are likely to be inaccurate for safety-critical software.
5. The empirical results indicate that: for safety-critical software, the required safety can be achieved by improving the reliability; however the vice-versa is not always true.

5. Conclusion

The methods and analysis presented in this thesis demonstrate the use of software testing to arrive at an estimate of the software reliability. The results on relationship between the software reliability and safety in safety-critical systems would be helpful in understanding the dynamics behind developing safer software based systems.

The proposed approaches can be used by safety-critical software developers to improve the software reliability. Also, the regulators may use the techniques to verify reliability, safety, and dependability claims.

Publications

Journals

1) An intuitive approach to determine test adequacy in safety-critical software, P. Arun Babu, C. Senthil Kumar, N. Murali, and T. Jayakumar, ACM Sigsoft software engineering notes, Volume 37, Issue 5 (Sept. 2012).
2) A hybrid approach to quantify software reliability in safety systems of nuclear reactors, P. Arun Babu, C. Senthil Kumar, and N. Murali, Annals of nuclear energy, Volume 50, December 2012, Pages 133-140.
3) Properties of software reliability in safety systems of nuclear reactors, P. Arun Babu, C. Senthil Kumar, N. Murali, and T. Jayakumar, Manuscript under review in Journal of systems and software.

Conferences/Symposiums/Articles

4) Software reliability in safety-critical applications:mA case study from the nuclear industry, P. Arun Babu, C. Senthil Kumar, N. Murali and T. Jayakumar, International Applied Reliability Symposium, Chennai, India, Oct. 2012.
5) Making formal software specification easy,P. Arun Babu, N. Murali, P. Swaminathan, and C. Senthil Kumar, 2nd International Conference on Reliability, Safety and Hazard, pages 511–516, Dec. 2010. doi: 10.1109/ICRESH.2010.5779603.
6) Semi-formal property verification in games, P. Arun Babu and N. Murali,Testing Experience, issue 15, pages 14–17, Sept. 2011.

Int ernal reports

Versions of the above publications have also appeared in the following internal reports:
1) A hybrid approach to quantify software reliability in safety systems AERB/SRI/2012/2007
2) Method to determine adequacy of software testing for reliability estimation of computer based systems in NPPs AERB/SRI/2013/2010
3) Development of software reliability assessment methodology using model and mutation based testing for systems important to safety in FBRs EIRSG/ICG/RTSD/PRIS(G)/2012-13/IV(8a)
4) Test case adequacy assessment using mutation based testing and test coverage for computer based safety related systems in FBRs EIRSG/ICG/RTSD/PRIS(G)/2012-13/IV(8b)

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Title	:	Electromagnetic and Hard Probes of Strongly Interacting Matter

Abstract

The thesis contains theoretical investigations associated with the extreme state of matter, called Quark-Gluon Plasma (QGP), which is created in the collisions of heavy nuclei at relativistic energies in the laboratory. Different aspects of QGP have been inspected through: Direct photon momentum correlation, Quenching of large momentum jets and Jet-triggered Compton back-scattered photon production in this work.

Within the framework of hadron resonance gas model, we have constructed an equation of state (EoS) of hot hadronic matter which consists of discrete hadronic states of mass (m)≤ 2 GeV and continuous Hagedorn states in the mass range 2< m< 12 GeV and accounted for the finite volume

of hadrons. This description is then switched over either to Bag model EoS or lattice EoS of QGP at temperature 165 MeV. The EoS includes the Bag Model admits a first order phase transition whereas the lattice based EoS shows a rapid cross-over from QGP to hadron gas. Using the two EoS, we have calculated thermal particle and photon momentum spectra for the central collisions of gold or lead nuclei at the top RHIC (200A GeV) and LHC (5.5A TeV) energy respectively. The particle and photon spectra have shown marginal sensitivity to the difference between the two EoS. However the thermal photon intensity correlation has been found to be quite distinct for the two EoS, especially for the outward direction. Thus the work could be proved valuable in respect of probing the EoS of strongly interacting matter in experiment.

We have investigated the system size dependence of jet-quenching by analyzing the suppressed production of hadrons in the collisions of gold and copper nuclei at RHIC (200A) and lead nuclei at the LHC (2.76A TeV) energy. Next-to leading order perturbative quantum chromodynamics has been used for the initial production of partons and then they are assumed to lose energy via gluon radiation while traversing the QGP. The energy loss per collision, ε, is taken proportional to the energy of the parton (E), √E or constant for the incoherent, partial coherent and complete coherent regimes of gluon radiation. The probability of multiple scattering of partons and nuclear modification to the parton distributions are also taken into account. The QGP medium is considered as an assembly of static scattering centers at some fixed temperature. By treating ε as the only free parameter, we have reproduced the centrality dependence of nuclear modification factor (R_{AA}) of hadron production measured at RHIC and LHC experiment. Thus the work has demonstrated the change in parton energy loss mechanisms which is reflected through the transverse momenta of final state hadrons.
The direct photons (real and virtual) are considered as an excellent messenger of QGP properties because of their weak electromagnetic coupling with the medium. Several sources of direct photon have been proposed so far in theory but separation of a single contribution is a challenging task in experiment. The jet-medium Compton back-scattered photons are found to contain valuable information about the temperature and parton energy loss mechanism in QGP. We have proposed a novel way to separate these photons from other direct photon sources by using the correlation with a trigger jet at large photon momentum. Only the hard prompt photons are produced in coincidence with a jet, hence considered as a 'background' for this study. We have evaluated the invariant yield and nuclear modification factor (R_{AA}) of back-scattering photons in coincidence with the trigger jet at leading order of strong coupling for the central collisions of gold or lead nuclei at RHIC (200A GeV) and LHC (2.76A TeV) energy. The back-scattering photons have caused a sharp peak in R_{AA} around the trigger jet window which could be considered as potential signal. However it has been found that inclusion of higher order processes for the 'background' and account for the trigger jet energy loss tends to wash out the signal. Thus we conclude that there exists a possibility to separate back-scattering photons from other sources if the energy of the trigger jet can be determined reliably in experiment.

Publications

a. Published:

In Journals:

1) Equation of state of strongly interacting matter: spectra for thermal particles and intensity correlation of thermal photons. S. De, D. K. Srivastava and R. Chatterjee, J. Phys. G 37, 115004 (2010).
2) System size dependence of nuclear modification and azimuthal anisotropy of jet quenching. S. De and D. K. Srivastava, J. Phys. G 39, 015001 (2012); Corrigendum: J. Phys. G 40, 049502 (2013).
3) Nuclear modification of charged hadron production at LHC. S. De and D. K. Srivastava, J. Phys. G 40, 075106 (2013).

4) Predictions for p+Pb collisions at $\sqrt{s_{NN}}$ = 5 TeV*. J. L. Albacete et al., Review paper 6.1 Direct photon cross-section, R. J. Fries and S. De International J. of Mod. Phys. E 22, 1330007 (2013).

In conference/ symposium proceedings:

1) Equation of state of strongly interacting matter and intensity interferometry of thermal photons. S. De, D. K. Srivastava and R. Chatterjee, Nucl. Phys. A 862-863 (2011) 290c-293c. 6th International Conference on Physics and Astrophysics of Quark Gluon Plasma, 6-10 December, Goa, India.
2) Centrality dependence of jet-quenching at RHIC. S. De and D. K. Srivastava Proceedings of the DAE Symposium on Nucl. Phys. 56, 906-907 (2011).
3) Jet-Tagged Back-Scattering Photons for Quark Gluon Plasma Tomography. R. J. Fries, S. De, D. K. Srivastava, Nucl. Phys. A 904-905 (2013) 569c-573c. Quark Matter 2012 International Conference, 13-18th August, Washington DC, USA.
4) Jet-Tagged Back-Scattering photons for Quark Gluon Plasma Tomography. R. J. Fries, S. De, D. K. Srivastava, Nucl. Phys. A 910-911 (2013) 482c-485c. Hard Probes 2012, 27 May- 1 June, Cagliari, Italy.

b. Accepted:

1. Extent of sensitivity of single photon production to parton distribution functions*.
2. S. De, arXiv: 1305.0624, To appear in Pramana, Journal of Physics.
3. Centrality dependence of nuclear modification factor at RHIC and LHC.S. De and D. K. Srivastava, To appear in the proceedings of QGP meet-2012, 3-6 July, VECC, Kolkata.

c. Communicated:

1. Jet-Triggered Back-scattering Photons for Quark Gluon Plasma Tomography. S. De, R. J. Fries, and D. K. Srivastava, arXiv: 1402.1568.

(*) These works are not included in the thesis.

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Title	:	Pattern Formation in Complex Systems

Abstract

This thesis is a study of emergent spatiotemporal patterns in an extended system of interactive dynamical elements, under varying nodal dynamics and coupling architectures. In here, we have incorporated a range of complexity, in both nodal dynamics and connections and studied their role on the emergent spatiotemporal behavior of the extended system.

We have addressed the effect of various complexity classes on spatiotemporal dynamics of an extended system using the framework of coupled maps and coupled oscillators. There are five main problems which have been addressed in each of the main Chapters in the thesis:

(i) The role played by positive and negative links on spatiotemporal regularity of a random weighted neuronal network: we have found regularity in this network when the connections weights are predominantly positive or negative. However, for balanced connections we observed spatiotemporal chaos in the network.

(ii) Effect of coupling heterogeneity on the formation of clusters in a coupled neuronal lattice:

we found that not only the coupling heterogeneity but also a particular type of coupling architecture is needed for a particular pattern.

(iii) How does the synchrony of a subpopulation depends on inter/intra-group connection weights, relative size of the groups and their intrinsic dynamical behavior in a coupled neuronal population through group interaction? We observed that, synchronization is crucially dependent on the relative sizes of the interacting sub-populations.

(iv) Effect of parametric heterogeneity present at the nodal level and the random connections in a coupled neuronal population on the temporal regularity of spikes events: we found that largest coherence in the spike events for this network emerge when the coupling strength is large, and the underlying connections are mostly random and dynamically changing.
(v) Effect of delayed connection and boundary condition on spatiotemporal patterns in an array of chemical oscillators: we observed that spatiotemporal patterns are dependent on the boundary conditions. Also, the phenomena of oscillation death is only observed in non-delayed case whereas anti-phase patterns are only observed in delayed case.

Publications

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5. nterplay of diversity and random connection on coupled neuronal populations. N. K. Kamal, S. Sinha.

Name	:	**Sudhanshu Shekhar Pati**
Enrolment No.	:	CHEM02200804010
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Title	:	Synthesis and Characterization of Magnetic Nanoparticles with Enhanced Thermal Stability

Abstract

Superparamagnetic ferrite nanoparticles and their dispersions have been a topic of intense research for the last few decades because of their practical applications. Irrespective of the advances in this field, preparation of magnetic nanomaterials with high thermal stability and desirable saturation magnetization still remains as a challenge. Further, for effective utilization of ferrite nanoparticles for practical applications, control on polydispersity, purity and magnetization are necessary. Due to ferrimagnetic to antiferromagnetic phase transition of Fe_3O_4 nanoparticles, the applications of these nanoparticles are limited to ~ 500 ^{0}C. The major objectives of the present study was to develop methodologies to enhance the high temperature phase stability of magnetite nanoparticles, to obtain insight into the effect of cation doping on thermal stability and magnetic properties of magnetite nanoparticles and to study the effect of reaction temperatures on high temperature phase stability of magnetite nanoparticles.

It has been found that the thermal stability of Fe3O4 nanoparticles can be dramatically enhanced by doping it with a low concentration of Co, Zn and Na. Under air atmosphere, the maghemite to hematite phase transition is enhanced by 100 °C with 0.1 fraction of Co. The enthalpy change during the y-Fe_2O_3 to a-Fe_2O_3 phase transition decreases from 90 to 17 J/g as the Co fraction is

increased from 0 to 0.6, which indicates that the degree of conversion from maghemite to hematite decreases with the Co content. Under air atmosphere, the magnetic phase (y-Fe_2O_3) is retained till 656 °C with 0.6 fraction of Zn doping. The saturation magnetization increases from 61 to 69 emu/g when doped with 0.2 fraction of Zn.

The Na doping in Fe_3O_4 nanoparticles confirms that y-Fe_2O_3 to a-Fe_2O_3 phase transition temperature increases with Na+. The zeta potential results indicate that the Na+ ions are diffused into the crystal lattice. In situ XRD study, under vacuum annealing, on Zn doped Fe_3O_4 system shows that 0.2 fraction of Zn doping can enhance the phase transformation temperature of Fe_3O_4 by ~300 °C. The spinel ferrite phase is found to be stable upto 1000 °C, when doped with 0.1 fraction of Co. Under vacuum annealing, no phase transition is observed up to 1000 °C in Fe_3O_4 nanoparticles doped with 500 ppm of Na.

Phase pure magnetite nanoparticles of size raging from 7-10 nm are prepared by varying the reaction temperature from 50 to 200 °C, using microwave assisted method. The average particle size obtained from SAXS is found to vary from 11 to 15±1 nm as the reaction temperature is increased from 50 to 200 °C. The ferromagnetic y-Fe_2O_3 to antiferromagnetic a- Fe2O3 phase transition temperature is found to increase by 154 °C in the sample prepared at 200 °C, which is attributed to the diffusion of Na+ within the cubic lattice during synthesis.

Microwave assisted synthesis method has been successfully used to prepare $Mn_xZn_{1-x}Fe_2O_4$ nanoparticles. The Curie point was found to increase linearly from 148 to 390 K as the Mn fraction is increased from 0.1 to 0.55. The results showed that by varying the relative fraction of Mn and Zn in ferrite structure, the particle size, lattice parameter, Curie temperature and the magnetic properties of Mn-Zn ferrites can be tuned.
Publications

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6. "Synthesis of $Mn_xZn_{1-x}Fe_2O_4$ Nanoparticles with Tunable Curie Temperature using Microwave Assisted Method", S. S. Pati, S. Kalyani, V. Mahendran and J. Philip (Under review).

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2. Conference on chemistry in societal and environmental needs held at Central Leather Research Institute, Chennai, Aug 29-31(2011).

3. S. S. Pati and John Philip, "Enhancement in maghemite to hematite phase transition temperature with very low fraction of Co (II) doping", International Conference on Nanoscience Engineering and Technology (ICONSET), Sathyabhama University, Chennai Nov 28-30 (2011), pp 323-325.

Name	:	**Nageshwar Singh**
Enrolment No.	:	PHYS03201004004
Date of Award of degree	:	10.07.14
Constituent Institute	:	Raja Ramanna Centre for Advanced Technology, Indore
Title	:	Studies on Narrow Bandwidth High Repetition Rate Dye Laser

Abstract

Spectral stability a narrow bandwidth high repetition rate dye laser has been a major area of research work over the years. With this in view, crucial factors such as dye cell geometries and dye gain medium flow, which influence the spectral characteristics of copper vapour laser (CVL) pumped Rhodamine 6G (Rh6G) dye laser, are investigated for the thesis work. Overall, the thesis focuses spectral stability of high repetition rate dye laser and in particular, studies on dye cells, dye laser gain medium flow, diagnostics techniques, pulsed dye laser resonator and other related thermo-optic issues. For these purposes, new dye cells of different geometries such as curved, pinched, convex-plano were designed and fabricated. The velocity profiles through the pinched and convex-plano geometries were numerically analyzed, using computational fluid dynamics. A special dye circulation and cooling system was designed, fabricated and incorporated into high repetition rate dye laser system. A novel diagnostic technique for a large number of data acquisition, presentation, and its precise measurements were formulated and effectively executed to explore the dye laser spectral characteristics, over a period of time. The dispersion theory for narrow bandwidth pulsed dye laser analyzed theoretically and numerically. The dye laser resonator was investigated for maximum optical power extraction. Single mode operation of dye laser was experimentally demonstrated. The dye laser spectral stability was investigated using the dye cells developed. The dye laser gain medium thermal and flow characteristics as a function of Reynolds number were investigated. The dye laser spectral fluctuations as a function of Reynolds number were investigated. The dye fluorescence fluctuations in stationary as well as in the flowing media have been experimentally investigated. The dye laser thermo-optical properties have been investigated.

The above and other related works have been published in various peered reviewed journals.

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1. "A study of flow characteristics of a high repetition rate dye laser gain medium", Nageshwar Singh, Abhay Kumar and H. S. Vora, Laser Physics, 2014, Vol.24, 025004-6
2. Studies on gain medium inhomogeneity and spectral fluctuations coupled with high repetition rate dye laser", Nageshwar Singh, Abhay Kumar and H. S. Vora, Laser Physics, 2013, Vol.23, 125003-6
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4. "Spectral intensity variation by the correlation function of refractive index fluctuations of the liquid medium", Nageshwar Singh, International Journal of Optics, 2013, Vol.2013, 525142-7
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7. "Fluorescence fluctuation of Rhodamine 6G dye for high repetition rate laser excitation", Nageshwar Singh, H. K. Patel, S. K. Dixit and H. S. Vora, Journal of Luminescence, 2013, Vol.134, 607-613
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13. "Study of the influence of the input electric power on the spectral width of the 510.6 nm line of an atomic copper vapor laser", Nageshwar Singh and H. S. Vora, Optics & Laser Technology, 2010, Vol.42, 866-872
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8. "On the stability of the output characteristics of a grazing incidence grating dye laser transversely pumped by a copper vapor laser", Nageshwar Singh and H. S. Vora, Applied Physics B, 2006, Vol.82, 71-74
9. "Design of a transversely pumped, high repetition rate, narrow bandwidth dye laser with high wavelength stability", R. Bhatnagar, Nageshwar Singh, R. Chaube and H. S. Vora, Review of Scientific Instruments, 2004, Vol.75, 5126-5130

Name	:	**Ratika R. Kunder**
Enrolment No.	:	LIFE09200704010
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Constituent Institute	:	Tata Memorial Centre, Mumbai
Title	:	MicrorRNA Profile of Medulloblastomas

Abstract

Medulloblastoma, a tumor of the cerebellum, is the most common malignant pediatric brain tumor. It is thought to arise from deregulated nervous system development. MicroRNAs (miRNAs) are a class of non-coding RNA molecules that act as post-transcriptional regulators of gene expression. MiRNAs have been reported to play a critical role in cell proliferation, differentiation, stem cell maintenance and development. Altered miRNA expression has been reported in various cancers. Therefore, in order to gain a better understanding of medulloblastoma biology, miRNA profiling of medulloblastomas was carried out.

Medulloblastomas have recently been shown to comprise of 4 molecular subgroups viz. WNT, SHH, Group 3 and Group 4. MiRNA profiling revealed differential miRNA expression in these 4 molecular subgroups with the WNT subgroup having the most distinctive miRNA profile. The differential expression of 11 miRNAs across the 4 subgroups was validated in a total of 101 medulloblastomas by real time RT-PCR, which also confirmed the distinctive WNT subgroup miRNA profile. Functional role of 3 WNT subgroup specific miRNAs in medulloblastoma cell behavior was investigated wherein, miR-193a-3p was found to reduce proliferation, anchorage-independent growth and increase radiation sensitivity of medulloblastoma cells, indicating its therapeutic potential in the treatment of non-WNT medulloblastomas. A Real time PCR based assay for molecular classification of medulloblastomas using 12 protein-coding genes and 9 miRNAs was developed and validated on an independent cohort from DKFZ, Germany with known subgroup affiliation. This assay with an accuracy of 97 % could reliably classify formalin-fixed, paraffin-embedded medulloblastoma and has the potential to serve as a simple, rapid and cost-effective method in routine clinical diagnosis. Correlation of the miRNA profile data with clinical characteristics identified miR-592 and miR-182 as indicators of better and poorer survival respectively in case of non-WNT, non-SHH medulloblastomas. Since the assay includes oncogenes like MYC, MYCN as well as miRNAs like miR-592 and miR-182, it is also useful for risk stratification within the 4 subgroups. This is the first comprehensive study on medulloblastomas from the Indian subcontinent. Although the demographic profile of the Indian cohort was similar to that reported for the tumors from the American and European subcontinent, notable differences were seen. The Indian cohort showed a two-fold higher incidence of WNT subgroup tumors, absence of adult patients and high male: female ratio of 9:1 in Group 4 medulloblastomas.

Overall, the study not only demonstrated miRNAs as biomarkers for molecular classification and risk stratification of medulloblastoma but also indicated their role in pathogenesis and their therapeutic potential.

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2. "Outcome analysis based on clinico-pathologic factors and molecular sub-grouping in Indian patients with medulloblastoma treated on prospective clinical trials." Tejpal Gupta, Rahul Krishnatry, Neelam Shirsat, Sridhar Epari, Ratika Kunder, Purna Kurkure, Tushar Vora, Aliasgar Moiyadi and Rakesh Jalali. 15th International Symposium on Pediatric Neuro-Oncology, June 24-27 2012 Toronto, Ontario, Canada. Neuro Oncol. 2012; 14 (suppl 1):i82-i105.

Name	:	**Lakshmoji Kosuru**
Enrolment No.	:	PHYS02200804007
Date of Award of degree	:	11.07.14
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	On the Use of Silicon Microcantilevers for Mass Detection and Adsorption of Water Molecules

Abstract

Present thesis deals with two important aspects of microcantilever (MC) based sensors. In the first part, methods to enhance the MC mass sensitivity are studied. Working at higher modes and reducing the dimensions of MC are compared. Resonance frequency of MC is measured using the laser photo diode arrangement of an Atomic Force Microscopy (AFM) head and Nano Vibration Analyzer (NVA). Micro-Raman spectroscopy was used to estimate the residual stress in MCs. Finite Element Modeling (FEM) analysis was extensively used to identify and assign the mode shapes of MC, obtained experimentally. A precise dip coating setup is indigenously developed to add polymer mass on MCs. It is shown that mass sensitivity increases linearly with increase of eigenvalue (λ_n^2) and decreasing dimensions (T/L^2) where T is thickness and L is length of MC. Using FEM simulations, mass sensitivities for various nanostructures like nanobelt, nanowire and nanotube which can be attached to a conventional MC are studied. Factors affecting the dynamic range of cantilever based mass sensors are discussed. Polymer (PAAM and PVP) coated MCs are also explored for gamma radiation dosimeter application.

In the second part of the thesis, resonance frequency shift upon adsorption of water molecules in MCs with reducing dimensions are investigated. AFM head placed inside an air tight chamber, purged with dry/wet N_2 is used for these studies. Experimental evidence has been presented to show that the effect of dimensions of MC leads to negative or positive frequency shift during adsorption, clearly depicting the competition between mass loading and stiffness changes. The relative change in stiffness of MC is seen to increase linearly with the surface stress scaled with cube of width to height ratio of MCs, confirming the dimensional dependence of adsorption induced stiffness change. Adsorption and desorption kinetics of water molecules on MC surface are studied. Apart from this, various possible mechanisms responsible for deflection of uncoated Si MC when exposed to water molecules is discussed. It is shown that the bending is a consequence of difference in surface roughness on front and back side of uncoated MCs. The results are explained in terms of the large number of "stress concentrators" on the back side compared to front side of MC in accordance with the recent theoretical models. Finally it is demonstrated that uncoated MCs can be effectively used as a humidity sensor both in static and dynamic mode.

Publications

a. Journal Publications

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2. K.Lakshmoji, K.Prabakar, Atul Kumar, J.Jayapandian and A.K.Tyagi, Enhancing the mass sensitivity of nanocantilever, International Journal of Nanoscience, Vo.11, No.1, 1250002, 2012.
3. K.Lakshmoji, K.Prabakar, R. Mythili, J.Jayapandian, Effect of UV light on the bending properties of piezoresistive microcantilevers, Proceedings of "International Conference on Nanoscience, Engineering and Technology (ICONSET 2011)" held at Sathyabama University, Chennai, IEEE Conf. series (December, 2011) 518 - 519.
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5. K.Lakshmoji, K.Prabakar, S. Tripura sundari, J.Jayapandian and C.S.Sundar, Effect of surface stress on microcantilever resonance frequency during water adsorption: influence of microcantilever dimensions (Ultramicroscopy, Accepted)

Name	:	**Ajit Kumar Sharma**
Enrolment No.	:	LIFE09200704009
Date of Award of degree	:	17.07.14
Constituent Institute	:	Tata Memorial Centre, Mumbai
Title	:	Histone, Chromatin Structure and their Role in DNA Repair During Carcinogenesis

Abstract

Chromatin acts as a natural barrier in DNA-damage recognition, repair and recovery. Histone and their variants undergo differential post-translational modification(s) and regulate chromatin structure to facilitate DNA damage response (DDR). Also, these histone marks are known to alter during cell cycle to maintain distinct chromatin states in specific phases of cell cycle. Therefore, cell cycle phase specific histone marks may be the key determinants for differential response of ionizing radiation in different phase of cell cycle. The aim of the present study is to investigate cell cycle phase specific alteration of histone marks and associated proteins in response to DNA damage.

In this study we have unravelled alteration in H3Serine10 phosphorylation (H3S10P) in response to ionization radiation (IR) induced DNA damage during cell cycle. Our data shows that H3S10P decreases specifically from irradiated G1-enriched cells in 'prime-repair' phase with restoration in 'recovery' phase of DDR, whereas H3S10P level remains unaltered in S, G2/M and pro-M phase cells after DNA damage. The pattern of H3S10P shows an inverse correlation with γH2AX during DNA damage response. Further, dephosphorylation of H3S10P is observed in multiple cell lines from different tissue origins and various DNA damaging agents concluding H3S10P as a universal G1-specific DNA damage responsive histone mark. The decrease in H3S10P in response to DNA damage is predominantly from H3.3 variant, a major H3 variant in G1 phase of cell cycle. Interestingly, our data report for the first time that de-phosphorylation of H3S10 occurs from the same mono-nucleosomes bearing γH2AX after DNA damage. The global chromatin compaction is observed during repair phase with restoration of native chromatin structure in 'recovery' phase of DDR. Collectively, our data identifies H3S10P as a first universal G1-phase specific DNA damage responsive histone mark and is inversely correlated with γH2AX, a DNA damage responsive mark.

The studies further unraveled regulation of H3S10P in response to IR-induced DNA damage in G1-phase of cell cycle. The dynamic reversible reduction of H3S10P is mediated by opposing activities of phosphatase, MKP1 and kinase, MSK1 of the MAP kinase pathway. MKP1, recruits to chromatin in response to DNA damage that correlates with decreased H3S10P, whereas MKP1 gets released from chromatin during recovery of damaged DNA which correlates with restoration of H3S10P level in G1 phase of cell cycle. The specific inhibitors against MKP1 and MSK1 confirms the dynamic alteration and association of enzymes with chromatin that regulate histone mark, H3S10P in response to DNA damage. Collectively, our data suggest that phosphorylation status of H3S10 is an essential G1-DNA damage responsive histone mark along with γH2AX for maintaining the nucleosomal architecture for efficient recognition, repair and recovery of DNA lesion.

Publications

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2. Rhea Mohan, Ajit K. Sharma, Sanjay Gupta, C. S. Ramaa. Design, synthesis, and biological evaluation of novel 2, 4-thiazolidinedione derivatives as histone deacetylase inhibitors targeting liver cancer cell line. Med. Chem. Research, March 2011, pp, 1-10.
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Name	:	**O. Annalakshmi**
Enrolment No.	:	PHYS02200704007
Date of Award of degree	:	18.07.14
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	Dosimetric Characteristics of Borate Based Thermoluminescent Materials

Abstract

Thermoluminescence (TL) dosimetry is a widely used means of radiation dosimetric measurements, especially for personnel and environmental monitoring. The energy of the ionizing radiation is absorbed by thermoluminescent materials and some part of the absorbed energy is stored in defect centers (trapped electrons and holes, radicals, displaced ions). In thermoluminescence dosimetry, the stored energy is released in the form of light by thermal stimulation, with the amount of light proportional to the amount of absorbed radiation energy (absorbed radiation dose).

Luminescent detectors of radiation should meet several requirements, such as low detection

threshold or high sensitivity, the absence of information losses in time (low fading), the absence of false-dose effects due to visible light and near ultraviolet radiation, a good linear dose response over a wide range of measurements and human tissue equivalence. Recently borate based phosphors are gaining more importance because of the ease of synthesis in bulk quantites, simple glow curve structure, increased neutron and gamma sensitivity, near tissue equivalence in some cases.

This thesis presents detailed dosimetric studies of borate based phosphors. Four borate based phosphors, viz., lithium tetraborate, magnesium tetraborate, zinc metaborate and cadmium tetraborate have been synthesized by solid state diffusion technique and their dosimetric properties are characterized for its crystallographic and thermoluminescence properties. The kinetic parameters of the TL glow curves (like trap depth, order of kinetics and frequency factor) for all the above phosphors were also evaluated by different methods. In addition, an attempt has been made for the first time to elucidate the mechanism of TL in each of the above phosphors using electron paramagnetic resonance (EPR) studies. Further, the scope for the future work is also discussed.

Publications

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8. O. Annalakshmi, M.T. Jose, J. Sridevi, B. Venkatraman G. Amarendra and A.B. Mandal, Kinetic parameters and TL mechanism in cadmium tetraborate phosphors, Journal of Luminescence, Vol - 147, (2014), 284-289

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1. O. Annalakshmi, M.T. Jose. S.R. Anishia and G. Amarendra, Dosimetric studies on tissue equivalent TL phosphor $Li_2B_4O_7$:Mn, Proceedings of NCLA -2009, Feb 18- 20, 2009, Kolkata
2. O. Annalakshmi, S.R. Anishia and M.T. Jose, Luminescence studies in cadmium borate TL phosphor, National conference on Luminescence and its applications on Feb 9-11, 2010 held at Gandhigram Rural Institute, Gandhigram, Tamilnadu
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1. A. R. Lakshmanan, M. T. Jose, and O. Annalakshmi, High-sensitive $CaSO_4$:Dy thermoluminescent phosphor synthesis by co-precipitation technique, Radiat Prot Dosimetry (2008) 132 (1): 42-50
2. S.R. Anishia, M.T. Jose, O. Annalakshmi, V. Ponnusamy and V. Ramasamy, Dosimetric properties of rare earth doped $LiCaBO_3$ thermoluminescence phosphors, Journal of luminescence, Vol -130, (2010), 1834-1840
3. S.R. Anishia, M.T. Jose, O. Annalakshmi, and V. Ramasamy, Thermoluminescence properties of rare earth doped lithium magnesium borate phosphors, Journal of luminescence, Vol -131, (2011), 2492 -2498
4. M.T. Jose, S.R. Anishia, O.Annalakshmi, V. Ramasamy, Determination of thermoluminescence kinetic parameters of thulium doped lithium calcium borate, Journal of luminescence, Vol - 46 (2011), 1026 - 1032
5. O. Annalakshmi, M. T. Jose, and U. Madhusoodanan, Synthesis and characterisation of $BaSO_4$:Eu thermoluminescence phosphor Radiat Prot Dosimetry (2012) 150 (2): 127-133
6. O. Annalakshmi, Varghese Anto Chirayath, S. Hari Babu, M. T. Jose, G. Amarendra, Positron lifetime studies of $CaSO_4$:Dy thermoluminescence phosphors, Physica Status Solidi (C), Vol - 6, (2009) 2516 - 2518

Publications in Conferences not included in thesis

1. S.R. Anishia, M.T. Jose, O. Annalakshmi, and V. Ponnusawmy, Dosimetric Characteristics of LiCaBO3Thermoluminescence Phosphor, Proceeding of NCLA -2009, Feb 18- 20, 2009, Kolkata
2. O. Annalakshmi, M.T. Jose and G. Amarendra, Thermoluminescence and Photo luminescence Studies on $BaSO_4$:Eu Phosphor, Proceeding of NCLA -2009, Feb 18- 20, 2009, Kolkata
3. S.R. Anishia, O. Annalakshmi and M.T Jose, Thermo luminescence properties of lithium magnesium borate phosphor, National conference of Luminescence and its applications on Feb 9-11, 2010 held at Gandhigram Rural Institute, Gandhigram, Tamilnadu

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Title	:	Structural Studies on Geometrically Frustrated Systems : AIV2O4 and LiMn2O4 - Role of Temperature, Pressure and Chemical Substitution

Abstract

Whenever a conflict arises between some fundamental interaction and the underlying lattice geometry, a geometrical frustration is said to result. The effect of such a geometrical frustration can be one of the following: finite entropy at zero Kelvin (degenerate ground state) or relieving of the frustration through a structural transition. The B sub-lattice of a spinel system (AB_2O_4, Fd-3m) made of corner sharing tetrahedra (pyrochlore lattice) is inherently geometrically frustrated. When this lattice is occupied by a multiple valent ion then there is charge frustration. There are just five spinel systems known so far that show ordering of charges from frustration. They are Fe_3O_4, $LiMn_2O_4$, $CuIr_2S_4$, AlV_2O_4 and $LiRh_2O_4$. In the present study two of them namely AlV_2O_4 and $LiMn_2O_4$ have been chosen and the role of pressure, temperature and B site substitution with respect to ordering of charges is examined.

From the study carried out in the present thesis, it is observed that the rhombohedral (charge ordered) to cubic (frustrated) structural transition occurs between 763 K-773 K in the case of AlV_2O_4. Pressure of about 20 GPa also destabilizes the 'heptamer' vanadium clusters formed due to the bonding interaction of d_{xy} orbitals. The electron energy loss spectroscopic measurements point out a novel non-integral charge state on all vanadium ions in the charge ordered structure. Instead of an external pressure internal pressure is altered by substituting Ru for Mn in $LiMn_2O_4$. Pristine $LiMn_2O_4$ shows partial ordering of Mn charges around 290 K. For samples with Ru more than 3.75%, low temperature resistance studies show absence of jump in the resistance associated with structural transition to partially charge ordered phase. On the contrary, low temperature diffraction experiments have shown that the structural transition does not vanish but is suppressed till 5% substitution of Ru. Hence as pressure retains frustration in AlV_2O_4, partial substitution for B sub-lattice too retains frustration down to 240 K. Further experiments are proposed to understand the nature of orbital ordering in these systems.

Publications

1. Pressure-induced frustration in charge ordered spinel AlV_2O_4 S. Kalavathi, Selva Vennila Raju, Quentin Williams, P.Ch. Sahu, V. S. Sastry and H. K. Sahu Fast Track Communication: J. Phys.: Condens. Matter 25 (2013) 292201
2. Synthesis, Characterization and Observation of Structural. Transformation in AlV_2O_4 S. Kalavathi, B. Thamilarasi, H. K. Sahu and V.S. Sastry AIP Conference Proceedings 1349 (2011) 1307
3. Valence state, hybridization and electronic band structure in the charge ordered AlV_2O_4 S. Kalavathi, S. Amirthapandian, Sharat Chandra, P. Ch. Sahu and H. K. Sahu J. Phys.: Condens. Matter 26 (2014) 015601

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Title	:	Corrosion Behaviour of Materials for the Nuclear High Level Waste Storage Application

Abstract

The main objective of the present investigation is to study the corrosion behaviour of new materials proposed for nuclear high level waste (HLW) storage application. Corrosion studies were carried out on three nickel based superalloys (Alloy 600, 690 and 693) in synthetic HLW solution simulated with fission and corrosion product elements in 3 M HNO3 using electrochemical techniques like potentiodynamic anodic polarization and electrochemical impedance spectroscopy. A comparison was made on the corrosion resistance of the superalloys under various conditions like as-received, solution-annealed, sensitized and laser surface melted treatment. Pitting corrosion resistance and intergranular corrosion resistance of these materials was also compared using the electrochemical techniques.

All the alloys, in the as-received and heat treated condition were found to possess good corrosion resistance in simulated HLW. X-ray photoelectron spectroscopic studies showed that the passive films formed on the Alloy 690 and Alloy 693 consists of a mixed oxide of Ni-Cr-Fe in simulated HLW, whereas only oxides of Cr could be observed in Alloy 600.

Laser surface melting of the Ni alloys resulted in cellular microstructure without any precipitates. These alloys found to possess same crystal structure (cubic) in both as-received as well as LSM

condition. Laser surface melting resulted in the enhancement of corrosion resistance of the alloys in simulated HLW compared to the as-received and solution-annelaed specimens; nevertheless, no discernable difference could be observed between LSM Alloys 600, 690 and 693 in simulated HLW.

The DL-EPR test was carried for all the heat treated and laser surface melted specimens in 0.5 M H_2SO_4 containing 0.0001 M KSCN. The LSM specimens showed very low DOS. Alloy 690 was found to contain no reactivation peak, due to the high chromium concentration.

From the Huey test, Alloy 690 was found to possess excellent IGC resistance compared to Alloy 600 and Alloy 693, which could be attributed to the higher chromium and lower carbon content. Studies were undertaken to evaluate the pitting corrosion resistance of the alloys in all conditions (as-received, solution annealed, sensitized and laser surface melted) in 3 M HNO3 containing various concentrations of chloride ions (500, 1000, 2000 and 3000 ppm) under aerated condition. A decrease in pitting corrosion resistance with increased chloride ion concentration was observed for all the alloys. The population of pits was also observed to increase with chloride ion concentration. Alloy 690 was found to possess superior pitting corrosion resistance compared to Alloy 693 and Alloy 600. The LSM specimens showed better pitting corrosion resistance in compared to the as-received and SA specimens, due to the refinement of microstructure and dissolution of precipitates, which are the initiation sites for pitting. Superior pitting corrosion resistance was exhibited by LSM Alloy 690 when compared to Alloy 600 and 693.

Publications

Journal

1) "Corrosion behavior of Alloy 690 and Alloy 693 in simulated nuclear high level waste medium", Pradeep Kumar Samantaroy, Girija Suresh, Ranita Paul, U. Kamachi Mudali and Baldev Raj, Journal of Nuclear Materials, 2011, 418, 27-37.
2) "Effect of heat treatment on corrosion behavior of Alloy 690 and Alloy 693 in simulated nuclear high-level waste medium", Pradeep Kumar Samantaroy, Girija Suresh and U. Kamachi Mudali, Corrosion, 2012, 68, 046001-1-046001-13.
3) "Corrosion behavior of Alloy 600 in simulated nuclear high level waste medium", Pradeep Kumar Samantaroy, Girija Suresh, N. G. Krishna and U. Kamachi Mudali, Journal of Materials Engineering and Performance, 2013, 22, 1041-1053.
4) "Corrosion enhancement of Ni base superalloys by laser surface melting", Pradeep Kumar Samantaroy, Girija Suresh, Rakesh Kaul and U. Kamachi Mudali, Surface Engineering, 2013, 29, 522-530.
5) "Effect of heat treatment on pitting corrosion resistance of nickel based superalloys in acidic chloride medium", Pradeep Kumar Samantaroy, Girija Suresh and U. Kamachi Mudali, International Journal of Material Science, 2013, 3,170-178.
6) "Corrosion investigation of nickel base superalloys in simulated high level waste medium using electrochemical impedance spectroscopy", Pradeep Kumar Samantaroy, Girija Suresh and U. Kamachi Mudali, (communicated).
7) "Intergranular corrosion behavior of nickel base superalloys", Pradeep Kumar Samantaroy, Girija Suresh, T. Nandakumar and U. Kamachi Mudali, (to be communicated).

Conference Proceedings & Presentations:

1) Pradeep Kumar Samantaroy, Girija Suresh, Ranita Paul and U. Kamachi Mudali, "Corrosion resistance of Ni 690 and Ni 693 in simulated nuclear high level waste", edited by T.S. Sudarshan, U. Kamachi Mudali and Baldev Raj, Surface Modification Technology, XXIII (2009), pp. 353-360.
2) Pradeep Kumar Samantaroy, Girija Suresh and U. Kamachi Mudali, Effect of heat treatment on corrosion behavior of Alloy 690 and Alloy 693 in simulated nuclear high level waste medium, International Conference on Advanced Materials - 2011 (ICAM-2011), Coimbatore, Dec. (2011).

3) Pradeep Kumar Samantaroy, Girija Suresh and U. Kamachi Mudali, "Pitting corrosion behavior of heat treated nickel base superalloys in acidic chloride medium", 16th National Congress on Corrosion Control (16th NCCC), Kolkata, India, Aug. (2012).
4) Pradeep Kumar Samantaroy, Girija Suresh, Rakesh Kaul and U. Kamachi Mudali, "Corrosion behavior of laser surface melted nickel base superalloys in simulated nuclear high level waste medium", 16th Asian Pacific Corrosion Control Conference (16th APCCC), Kaohsiung, Taiwan, Oct. (2012).
5) Pradeep Kumar Samantaroy, Girija Suresh, U. Kamachi Mudali, "Studies on nickel base superalloys for nuclear high level waste storage application", International Corrosion Prevention Symposium for Research Scholars (CORSYM-2013), Chennai, India, 28 Feb-02 Mar (2013).

Awards

1) 1st Prize for Oral Presentation: Pradeep Kumar Samantaroy, Girija Suresh and U. Kamachi Mudali, "Pitting corrosion behavior of heat treated nickel base superalloys in acidic chloride medium", 16th National Congress on Corrosion Control (16th NCCC), Kolkata, India, Aug. (2012)

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Title	:	X-Ray Spectroscopic Studies of Plasma Produced by Intense Laser Beams

Abstract

In this thesis work, a detailed x-ray spectroscopic study of the plasmas generated from nanosecond, picosecond and femtosecond laser pulses has been carried out to investigate the dynamics of x-ray emission. For carrying out the above x-ray spectroscopy work, the required x-ray spectroscopes were made in-house. An x-ray crystal spectrograph was made for high resolution measurements of the x-ray emission in the range of 1- 8 keV from the plasma. Dispersion-less spectrograph based on the x-ray CCD camera operation in single photon counting technique was designed, set up, characterized, and used in a variety of laser plasma experiment described in the thesis. It has been shown that x-ray emission from the plasma depends on the ionization equilibrium linked with the laser pulse duration. Next, a comparative study of the keV x-ray emission from gold-copper mix-Z targets of different atomic compositions has been carried out. The keV x-ray yield was observed to decrease even for a small fraction of gold in the mix–Z target.The results have been explained in terms of the enhanced absorption due to free–bound opacity, followed by down-conversion of the absorbed radiation. The x-ray emission from plasmas produced by the interaction of 45 fs Ti:sapphire laser pulses has been investigatedto understand the partition of energy between the thermal and non-thermal plasma.. The plasma conditions prevalent during the emission of x-ray spectrum have been identified by comparing the experimental spectra with the synthetic spectra generated using a spectroscopic code.

Next, tabletop, short-pulse laser-based 1-8 keV K-α x-rays source has been developed and characterized for the time resolved x-ray diffraction studies.The absolute yield of the K-α x-rays was measured as a function of the laser pulse duration and irradiation intensity.The results of optimal laser pulse duration for the maximization of K-α x-ray intensity have been explained in terms of efficient generation of optimal energy hot electrons due to trade-off between the electron energy and re-absorption of the emitted radiation in coming out of the target. We observed the spectral broadening K-α x-ray line shape and it has been attributed to the preformed plasma. A correlation of the spectral broadening K-$\alpha$with the 2ω and $3/2\ \omega$ emission harmonic in the optical spectrum is observed which can serve as a diagnostics for preformed

plasma. The source was utilized for studying the time resolved x-ray diffraction from a laser shocked silicon crystal with K-αx-ray probe. The dynamics of the strain propagation has been inferred by monitoring the evolution of the rocking curve width of the shocked sample at different time delays between the pump and the probe pulse.

Publications

A.Papers in refereed Journals :

1) Effect of gold on keV x-ray emission yield from laser produced plasma of gold copper mix-Z targets
V.Arora, J.A.Chakera, P.A.Naik, N.K.Gupta, S.R.Kumbhare, and P.D.Gupta
J. Appl. Phys. 100, 033306 (2006)
2) Study of 2 ω and 3/2ω harmonics in ultra-short high-intensity laser plasma interaction
V.Arora, P.A. Naik, J.A. Chakera, R.A. Khan, and P.D. Gupta
Pramana J. Phys. 75, 1175 (2010)
3) Conversion efficiency and spectral broadening of the K-α line emitted from planar titanium targets irradiated with ultra-short laser pulses of high intensity.
V.Arora, H. Singhal, P.A. Naik, and P.D. Gupta
J. Appl. Phys.110, 083305 (2011)
4) Strain and mosaic deformation in laser irradiated silicon.
M. Gupta, V.Arora, S. Bagchi, A. Gupta, J.A.Chakera, P.A.Naik, P.Chaddah, and P.D.Gupta.
Am. Inst. Phys. Conf. Proc. 1447, 785 (2011)
5) A comparative study of the ionic keV x-ray line emission from plasma produced by femtosecond, picosecond, and nanosecond duration laser pulses.
V.Arora, P. A. Naik, B. S. Rao, and P. D. Gupta
Pramana J. Phys.78, 227 (2012)
6) Laser induced shock studies at RRCAT, Indore.
P.A. Naik, V.Arora, S. Bagchi, Y.B.S.R. Prasad, S. Barnwal, and P.D. Gupta.
J. Physics: Conference Series 377,012052 (2012)
7) Dispersion-less spectrograph for absolute measurement of multi keV x-ray flux from highintensity laser produced plasmas
V.Arora, H.S. Vora, J.A. Chakera, M. Tayyab, P.A. Naik and P.D. Gupta
J. Instrum. 8, 01010 (2013)
8) Study of strain propagation in laser irradiated silicon crystal by time-resolved diffraction of K-α x-ray probe of different photon energies.
V.Arora, S. Bagchi, M. Gupta, J. A. Chakera, A. Gupta, P. A. Naik, P. Chaddah, and P.D. Gupta
J. Appl. Phys. 114, 023302 (2013)
9) Bright 1-8 keV K-α x-ray source generated by high intensity femtosecond laser produced plasma for time resolved x-ray diffraction studies.
V.Arora, P.A. Naik, J.A. Chakera, S. Bagchi, M. Tayyab, and P.D. Gupta
AIP Advances 4, 047106 (2014)
10) Spectral analysis of K-shell x-ray emission of magnesium plasma produced by ultra-short high intensity laser pulse irradiation.
V. Arora, U. Chakravarty, M. P Singh, J.A. Chakera, P.A. Naik, and P.D. Gupta
Pramana J. Phys.82, 365 (2014)

B. Publications in National Conferences/ Symposia:

1) X-ray CCD camera based crystal spectrograph for x-ray spectroscopy of laser produced plasmas
V.Arora, H. Singhal, P.A. Naik, U. Chakravarty, R.A .Khan, J.A. Chakera, R. Jain, H.S. Vora, and P.D.Gupta.
DAE-BRNS National Laser Symposium, (NLS-2006) Indore, Dec. 2006.
2) Optimization of the K-α radiation produced by interaction of high intensity femtosecond laser pulses with thick titanium foils.

V.Arora, H. Singhal, P.A. Naik, S.R. Kumbhare, and P.D. Gupta
DAE-BRNS National Laser Symposium, (NLS-2007) Vadodara, Dec. 2007.

3) Optimization of the K-α radiation produced by interaction of high intensity femtosecond laser pulses with thick titanium foils.
V.Arora, H. Singhal, P.A. Naik, S.R. Kumbhare, and P.D. Gupta.
DAE-BRNS National Laser Symposium, (NLS-2007) Vadodara, Dec. 2007.

4) Spectral broadening of K-α x-ray line emission from high-intensity ultra-short laser pulse irradiation of planar titanium targets.
V.Arora, H. Singhal, P.A. Naik, S.R. Kumbhare, and P.D. Gupta.
23rd National Symposium on Plasma Science and Technology, Mumbai, Dec. 2008.

5) X-ray radiation from the rear side of foil targets irradiated by ultra-short high intensity laser pulses
V.Arora, P.A. Naik, J.A. Chakera, S.R. Kumbhare, M. Tayyab, and P.D. Gupta.
24th National Symposium on Plasma Science & Technology, Hamirpur, Dec. 2009

6) Correlation of the K-α x-ray line shape with the 2ω and 3/2 ω emission in ultra-short high intensity laser plasma interaction.
V.Arora, P.A. Naik, J.A. Chakera, and P.D. Gupta.
International Symposium on Waves, Coherent Structures & Turbulence in Plasmas. Institute for Plasma Research, Gandhinagar. 12-15 January, 2010.

7) Spectroscopic study of laser light specularly reflected from solid targets irradiated by ultra-intense laser pulses.
V.Arora, P.A. Naik, J.A. Chakera, R.A. Ganeev, S.R. Kumbhare, and P.D. Gupta. DAE-BRNS National Laser Symposium (NLS-19), Indore, Dec. 2010

8) Study of shock wave propagation in silicon crystal by picosecond time-resolved x-ray diffraction.
V.Arora, S. Bagchi, R.A. Khan, M. Gupta, J. A. Chakera, A. Gupta, P. A. Naik, P. Chaddah, and P. D. Gupta.
26th National Symposium on Plasma Science & Technology, Patna, Dec. 2011.

9) Study of strain propagation in laser irradiated silicon crystal by time-resolved diffraction of K-α x-ray probe of different photon energies.
V.Arora, S. Bagchi, M. Gupta, J. A. Chakera, A. Gupta, P. A. Naik, P. Chaddah, and P. D .Gupta.
DAE-BRNS National Laser Symposium (NLS-20), Chennai, Jan. 2012.
(Awarded best poster prize)

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Title	:	Fused & Bridged Expanded Porphyrins and Expanded Calixphyrin : Structural Diversity and Receptor property

Abstract

Expanded porphyrins are macrocyclic compounds where pyrrole and / or heterocyclic rings are connected through meso-carbon bridges and show enhanced chemical and physical properties due to extended aromaticity. However, upon increasing the macrocycle size with more than six heterocyclic rings leads to deviation from planarity, which is mainly due to the intrinsic conformational distortion about meso positions. Suppression of the intrinsic twisting to figure eight structures is the challenge in the meso-aryl expanded porphyrins. The main objective of this thesis is to design a system which retains the planarity in solution and solid state; hence, one can use it for NLO applications. First part of the thesis describes the synthesis of bridged 1, 21 and fused 3, 42 expanded porphyrin systems.3 1 and 2 exhibit aromaticity with different π electron conjugation pathway. The fused derivatives 3 and 4 show protonation induced conformation change. Second part of the thesis demonstrates the synthesis, spectral, structural

characterization core-modified expanded calixphyrin (5)4 and their important properties such as; Aggregation induced enhanced emission and anion receptor properties.

Publications

1. Core-Modified meso-Aryl Hexaphyrins with an Internal Thiophene Bridge: Structure, Aromaticity, and Photodynamics Ganesan Karthik,Mahima Sneha, V. Prabhu Raja, Jong Min Lim, Dongho Kim, A. Srinivasan, and Tavarekere K. Chandrashekar
2. Calix[2]thia[4]phyrin: An Expanded Calixphyrin with AggregationInduced Enhanced Emission and Anion Receptor PropertiesGanesan Karthik, Pallavee Vitti Krushna, A. Srinivasan, and Tavarekere K. Chandrashekar
3. Conformational Change from a Twisted Figure-Eight to an Open-Extended Structure in Doubly Fused 36p Core-Modified Octaphyrins Triggered by Protonation: Implication on Photodynamics and Aromaticity Ganesan Karthik,Jong Min Lim, A. Srinivasan, C. H. Suresh, Dongho Kim, and Tavarekere K. Chandrashekar
4. Photophysical properties of bridged core-modified hexaphyrins: conjugational perturbation of thiophene bridges, Jong Min Lim, Karthik Ganesan, Young Mo Sung, Alagar Srinivasan, Tavarekere K. Chandrashekar and Dongho Kim
5. meso-Aryl Core-Modified Fused Sapphyrins: Syntheses and Structural Diversity Ganesan Karthik, A. Srinivasan, and Tavarekere K. Chandrashekar

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Title	:	Structural and Functional Characterization of BRCTs Domain

Abstract

Breast cancer is one of the common causes of death among women. Noting the growing number of breast cancer cases across the world, I decided to explore structures of the functional domains of the breast cancer gene product, BRCA1, specifically its BRCT domain. BRCT domains have long been documented as protein-protein interaction modules. The BRCA1 BRCT domain is inferred to be essential for BRCA1 to perform tumor suppressor functions, as it is found to be mutated in breast and ovarian cancers.

The protein-protein interactions are mediated through recognition, by BRCT domain, of a continuous stretch of amino acids containing the consensus sequences of S-X-X-F motif, and phosphorylated at one or two Ser residues. The singly phosphorylated binding partners are NCoA2, Nup153, RNA binding domain and Abraxas. Each of these selected proteins has different functions in association with the BRCT domain. Singly phosphorylated oligopeptides from these proteins are selected for structural and interactions studies. In the case of Abraxas, a doubly phosphorylated oligopeptide also is found to interact with the BRCA1 BRCT domain. The ITC analysis of these binding partners showed different binding affinities with BRCA1 BRCT. The crystal structures of BRCA1 BRCT complexed with NCoA2 and singly and doubly phosphorylated Abraxas peptides have been determined, by using the molecular replacement method. The BRCT-NCoA2 and BRCT-Abraxas singly phosphorylated peptide complex structures are determined at 1.7 Å and 3.5 Å resolution respectively. Crystallographic refinement of the structures revealed a “two knob” binding of both the oligopeptides with the BRCA1 BRCT domain. The phosphorylated Ser residue, pSer (0), is bound to N-terminal BRCT while Phe (+3) residue is inserted in the hydrophobic cleft formed at the interface region between the two BRCT domains.

The complex structure of BRCA1 BRCT with doubly phosphorylated Abraxas is determined at 3.8 Å resolution. In this structure the doubly phosphorylated Ser binds majorly to the N-terminal BRCT domain, with the pSer-404 rather than the expected pSer-406, occupying the phosphate binding pocket of BRCT domain. The cancer-associated BRCA1 H1686Q mutant is expressed and purified in a bacterial system. The CD and fluorescence spectroscopy analysis suggests that the secondary and tertiary structures are slightly changed upon mutation. Most of the other mutants, though expressed in bacterial system, but could not be purified in soluble forms. I, therefore, performed a molecular modeling analysis. The in-silico models of mutants predict alterations in the intramolecular hydrophobic interactions due to mis-sense mutations.

Publications

1. Badgujar DC, Sawant U, Mahadik H, Gadewal N, Varma AK (2012) Pathogenicity of Mutations Discovered in BRCA1 BRCT Domains is Characterized by Destabilizing the Hydrophobic Interactions. Journal of Cancer Science & Therapy 4: 386-393.
2. Badgujar DC, Sawant U, Yadav L, Hosur M, Varma AK (2013). Preliminary crystallographic studies of BRCA1 BRCT-ABRAXAS complex. Acta Crystallographica Section F: Structural Biology and Crystallization Communications 69: 1401-1404

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Constituent Institute	:	Bhabha Atomic Research Centre, Mumbai
Title	:	Studies on the Preparation and Characterization of U3Si2 Intermetallic and U-Mo Alloys

Abstract

Dispersion fuels are in general used for research and test reactors around the world and often termed as cold fuel. However there are reports available in the literature where its application in power reactors is also categorized. The concept/idea of dispersion fuel in Nuclear Reactor is very old. The examples of UO_2 dispersion in BeO matrix as the fuel elements for Daniels Pile experiment in 1946 and dispersion of UO_2 in stainless steel matrix as initial fuel for the first commercial power reactor licensed in United States in the year 1956 (e.g. Vallecitos Boiling Water Reactor) reiterates the fact. However the major application of dispersion type fuel elements remains for research and test reactors where HEU (High Enriched Uranium) based UAl_x compound is dispersed in aluminium matrix and clad with Al-alloy in plate type geometry around the world. However during mid 70's due to global concerns on proliferation the commerce in HEU based fuel was discouraged and international stipulation for LEU (Low Enriched Uranium) based fuel was formulated under RERTR (Reduced Enrichment for Research and Test Reactor) programme. The programme has now been put under the umbrella of GTRI (Global Threat Reduction Initiative) with broader objectives. The whole idea is to develop a fuel with higher fissile atom density so that loss of fissile atom enrichment can be compensated without affecting any major reactor core design.

In view of this and also keeping in line with the present International practice it was decided by the Department to fabricate the fuel core of modified APSARA indigenously on LEU. Hence a detailed fuel development activity with U_3Si_2 and U-Mo alloy as dispersoid in aluminium is included in the present study. These fuel compounds were prepared by an innovative powder metallurgy route with succinct intragranular porosity. The other advantage of synthesizing the compound/alloy by powder metallurgy route is getting a homogeneous product in single step with lesser impurity pickup since the processing temperatures are lower as compared with the melting casting route. Therefore for the synthesis of U_3Si_2 compound the starting powders of uranium and silicon were pressed together at high pressures (600 MPa) to induce plastic flow to

ensure intimate contact between powder particles. A small exothermic reaction ($\Delta H = -39.37$ kJ/mole at 750 °C) coupled with external heating was adequate to synthesize the compound. However, the product was deliberately heated in steps (i.e. 950 °C & 1400 °C) to accomplish the intended alloying reaction between uranium and silicon and also avoid any unalloyed phases. It was necessary to avoid bulk liquid formation in the process leading to inhomogeneous product. The product was finally heated at 1550 °C for 4 hours to complete the alloying to form the congruent melting compound well below its liquidus by taking advantage of mushy zone (liquid plus solid region shown in U-Si phase diagram).

However it is also understood that U_3Si_2 dispersoid in aluminium matrix can at best give heavy metal loading of 4.8 g/cm^3 which is insufficient for core conversion of ultra high power compact reactors. Hence another study on development and characterization of U-Mo alloy were carried out so that heavy metal loading in fuel meat can be increased to 8 to 9 g/cm^3. This study on U-Mo alloy preparation by powder metallurgy route showed that 2, 5 and 10wt% Mo concentration in uranium could be prepared with uranium and molybdenum metal powders as starting materials.
In addition to this the phase transformation study in U-Mo alloys was also carried out to study the effect of temperature on the stability of cubic □-phase of uranium. The study is relevant from the point of view that U-Mo alloy kernels are required to be coated by silicon by either CVD or PVD technique which requires them to be heat treated at around 450 to 500 □C. It was also observed that in case of U-Mo alloy particles dispersed in aluminium matrix, the chemical interaction between fuel granule and matrix will result in enveloping of fuel dispersoid by an intermediate phase. The interaction layer undergoes metamictization or becomes amorphous under irradiation and result in breakaway swelling. Since the free volume of the amorphous phase is highly compositional dependent therefore optimization of 'Mo' content in uranium to retain cubic □-phase under furnace cooling condition was also studied.

Publications

1. "Development of powder metallurgy technique for synthesis of U_3Si_2 dispersoid", V.P. Sinha,G.J. Prasad et.al. J. Nucl. Mater. 383(2008)196.]
2. "Development of high density uranium compounds and alloys as dispersion fuel for the research and test reactors", V.P. Sinha, G.J. Prasad et.al. Trans. Indian Inst. Met. Vol. 61, No. 2(2008), 1-6.
3. "Development, Preparation and Characterization of uranium molybdenum alloys for dispersion fuel application", V.P. Sinha, G.J. Prasad et.al. J. Alloys and Comp. 473(2009)238.
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Title	:	Dynamics of Heavy Quarks Produced in Relativistic Heavy Ion Collision

Abstract

We know that heavy ions colliding with relativistic energies may lead to the production of a very dense and thermally equilibrated system of quarks and gluons in a very small volume of space and for a very short time. Most of the contemporary works in this field is related to the studies of

this unique state called quark gluon plasma. My Thesis work is primarily related to heavy quark production in relativistic heavy ion collision and its evolution through quark gluon plasma. Because of its large mass as compared to infrared cut-off limit in QCD, its production rate can be controlled using perturbative techniques. Also we know that in heavy ion collision, heavy quarks are produced in early and preequilibrium stage when the interacting quarks and gluons possess large momenta. Some of the chapters in this thesis of my Ph.D. work deal with various heavy quark production mechanisms those can be realized and studied in heavy ion collision. The results show relative importance of these various mechanisms. Secondly heavy quark owing to its thermalization time greater than the typical lifetime of quark gluon plasma, remain isolated from bulk of the thermalized medium and hence it serves as a probe for the quark gluon plasma medium. The properties of the medium can be studied using heavy quark as probe via its energy loss and evolution of its properties while traveling through quark gluon plasma. Some of the chapters in my thesis deal with the studies of energy loss mechanisms and calculation of observables such as nuclear modification factor, R_{AA}, azimuthal anisotropy, V_2, and azimuthal correlation, C(A^) for heavy quarks. Also calculations related to heavy quark evolution using Boltzmann transport equation have been done and some transport coefficients and observables like momentum broadening, and medium path length dependence of heavy quark collisional and radiative energy loss have been calculated. Most of the results from the calculations done for this thesis work have been compared with the available data from heavy ion experiments being done at RHIC, BNL and LHC, CERN.

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• A manuscript titled "Charm Quark Energy Loss In Infinite QCD Matter Using Parton Cascade Model" is under final preparation by Mohammed Younus and co-authors Prof. Steffen A. Bass, Dr Dinesh K. Srivastava, and Christopher C-Smith has been submitted to Phys. Rev. C for review and publication. Preprints: arXiv:1309.1276v2 [nucl-th] 2013.

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Abstract

The statistical model has been often used to predict the distribution of evaporated particles from the excited compound nucleus populated by the energetic collision and subsequently the fusion of the target and the projectile. In statistical model, the particle emission probabilities are linked with the corresponding available phase spaces, which in turn are crucially dependent on the nuclear level density. An accurate determination of nuclear level density (NLD) and its dependence on excitation energy, atomic mass and angular momentum, is required to predict the cross-sections using statistical model. The dependence of level density on atomic mass and excitation are fairly well established. However, information available about the angular momentum dependence of level density is quite limited.

In the present thesis work, detailed experimental study of the angular momentum dependence of nuclear level density for the heavy nuclei in the mass region (A ~ 170 - 200) has been made by measuring the energy distribution of emitted neutrons in coincidence with y - ray multiplicity. The compound systems ^{169}Tm, ^{185}Re and ^{201}Tl have been populated at different excitations by the reactions ^{4}He + ^{165}Ho, ^{4}He + ^{181}Ta and ^{4}He + ^{197}Au respectively, using ^{4}He beams of 28 - 40 MeV energies from K130 cyclotron at VECC. Energy spectra of the evaporated neutrons have been measured in coincidence with the y -rays of different multiplicities (folds) using liquid - scintillator (BC501A) based neutron detectors through time of flight(TOF) technique and the y - multiplicity was measured using a 50 element BaF_2 based low energy y - ray filter array. It has been observed that the extracted level density parameter remained constant as angular momentum increases for all three systems at all excitation energies used in the present work. This trend is different from those observed in lighter systems, where NLD was found to be sensitive with the change in angular momentum. This findings open up prospects of detailed studies both theoretical and experimental on NLD over the whole mass range.

The present thesis is also devoted to the study on measurement and simulation of neutron response function of above mentioned neutron detectors , developed in - house. Neutron and y - ray pulse-height responses of the neutron detector were simulated using GEANT4 toolkit (version 4.9.2) and compared with experimental data in the energy range 2 - 20 MeV. The response functions of mono energetic neutrons of energies below 6 MeV have been extracted from the experimentally measured neutron energy spectrum obtained from the ^{252}Cf neutron source, and for energies > 6 MeV have been taken from the literature.

It was found that, for neutron energies <7 MeV, the measured response functions are well reproduced by GEANT4, but for energies >7MeV, GEANT4 could not predict the response functions properly. The reasons for discrepancies between the experimental and the GEANT4 simulated responses are due to the incompleteness of the physics processes NeutronHP model included in GEANT4 calculations. At higher neutron energies (E>8-10 MeV), higher order reaction channels like ^{12}C(n , a)^{9}B* ^ 2 a + n, ^{12}C(n , n') ^{12}C*^3 a become very important and should be properly taken into account.

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2. ''Angular momentum dependence of the nuclear level density parameter": M. Gohil, Pratap Roy, K. Banerjee, S. Bhattacharya, C. Bhattacharya, S. Kundu, T. K. Rana, T. K. Ghosh, G. Mukherjee, R. Pandey, J. K. Meena, H. Pai, V. Srivastava, A. Dey, Deepak Pandit, S. Mukhopadhyay, S. Pal, and S. R. Banerjee, EPJ web of conferences 66,03073(2014).
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3. ''Estimation of direct components of the decay of the Hoyle state": T. K. Rana, S. Bhattacharya, C. Bhattacharya, S. Kundu, K. Banerjee, T. K. Ghosh, G. Mukherjee, R. Pandey, P. Roy, V. Srivastava, M. Gohil, J. K. Meena, H. Pai, A. K. Saha, J. K. Sahoo, and R. M. Saha,

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4. "Study of angular momentum gated light-particle evaporation spectra in ^{4}He + ^{93}Nb and ^{4}He + ^{58}Ni reactions" : Pratap Roy, K. Banerjee, S. Kundu, T. K. Rana, T.K. Ghosh, C. Bhattacharya, G. Mukherjee, R. Pandey, J. K. Meena, M. Gohil, H. Pai, V. Srivastava, A. Dey, S. Mukhopadhyay, D. Pandit, S. Pal, S. R. Banerjee, and S. Bhattacharya, Proc. of DAE- BRNS symposium on Nucl. Phys. Vol. 57, 420 (2012). [2] [3] [4] Biswas, Proc. of DAE- BRNS symposium on Nucl. Phys. Vol. 57, 422 (2012).
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8. "Gamma ray spectroscopy of ^{197} Tl using a beam": H. Pai, G. Mukherjee, A. Goswami, S. Bhattacharyya, S. Chanda, T. Bhattacharjee, C. Bhattacharya, S. Bhattacharya, K. Banerjee, S. R. Banerjee, A. Chowdhury, P. Chowdhury, T. K. Ghosh, M. R. Gohil, S. Kundu, J.K. Meena, P. Mukhopadhyay, S. Mukhopadhyay, S. Pal, R. Pandey, D. Pandit, G. Prajapati,S. Rajbangshi , and T.K. Rana , Proc. of DAE- BRNS symposium on Nucl. Phys. Vol. 56 , 286 (2011).
9. ''Structure and decay mechanism of Hoyle state": T. K. Rana, S. Bhattacharya, Bhattacharya, S. Kundu, K. Banerjee, G. Mukherjee, J. K. Meena, R. Pandey, M. Gohil, H. Pai, A. Dey, T. K. Ghosh, M. Biswas, G. Prajapati, Proc. of DAE- BRNS symposium on Nucl. Phys. Vol. 56 , 492 (2011).
10. "Study of light-particle evaporation spectra (n, p, a) in ^{4}He+ ^{93}Nb 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, Proc. of DAE- BRNS symposium on Nucl. Phys. Vol. 56 , 540 (2011).
11. ''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, Pandit, S. Pal, S. R. Banerjee, and S. Bhattacharya, Proc. of DAE- BRNS symposium on Nucl. Phys. Vol. 56 , 594 (2011).
12. ''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, Proc. of DAE- BRNS symposium on Nucl. Phys. Vol. 55 (Part II), 324 (2010).

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Abstract

The main objective of the thesis has been to design novel molecular systems and materials for hydrogen energy applications using the available tools of computational chemistry. The studies are focussed on three important aspects of the hydrogen energy, viz. Hydrogen generation, its storage and effective usage in fuel cells. To generate hydrogen using the renewable solar energy through the photocatalytic water splitting, an appropriate photocatalyst is important. Through first principle studies, the thesis investigates s-triazine based graphitic carbon nitride and its non-metal doped counter parts as the possible metal- free photocatalyst to generate hydrogen. Hydrogen being light in weight, its storage with appropriate gravimetric and volumetric densities to use it as fuel is challenging. Through computational studies, it is shown here that the simple van der Waals surfaces are not capable of holding hydrogen efficiently and the presence of an ionic site can improve the adsorption considerably. Alkali metal decorated carbon and boron hydrides are explored as potential candidates for hydrogen adsorption and the stability of these systems has been correlated to the concept of aromaticity. Role of the curvature present in carbon nanomaterials towards alkali metal binding energy and hydrogen adsorption has been studied. Porous carbon nitride fullerene $C_{24}N_{24}$ has been shown to effectively bind with transition metal atoms and the metal decorated systems were reported to adsorb molecular hydrogen. Newly explored carbon allotropes, graphyne and graphdiyne were shown to be potential candidates for energy storage and nanoelectronics. Substitutional doping with boron in metal organic frameworks has been reported to improve the alkali metal binding as well as hydrogen

adsorption characteristics. New super cubane based three-dimensional porous carbon allotropes with different porosity were designed and their hydrogen adsorption characteristics were explored. In designing materials for fuel cell applications, we have explored the new catalysts for the oxygen reduction reaction, which is found to be the rate limiting step in fuel cell reaction. Transition metal (Fe, Co and Ni) decorated graphyne materials as well as the silicene based materials were shown to be effective catalyst for oxygen reduction reaction.

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Abstract

This thesis studies four problems on graphs using the Probabilistic Method. The first two are finding the maximum size of an induced acyclic tournament and acyclic subgraph respectively, in random directed graphs. The third one deals with finding the maximum size of an induced path, cycle or tree, in a random graph, while the last one is about an improved lower bound on the independence number of certain uniform hypergraphs.

Given a simple directed graph D = (V, A), let the size of the largest induced acyclic tournament be denoted by mat(D). Let D G D(n,p) (with p = p(n)) be a random instance, obtained by choosing each of the (n) possible undirected edges independently with probability 2p and then orienting each chosen edge in one of two possible directions with probability 1/2. We show that for such a random instance, mat(D) is asymptotically almost surely (a.a.s.) one of only 2 possible consecutive values, given explicitly as a function of p and n. Sufficient conditions for mat(D) to be 1-point concentrated are given. As a consequence, it is deduced that mat(D) is 1-point concentrated for all n belonging to a subset of positive integers of density 1 if p is independent of n. It is also shown that there are functions p = p(n) for which mat(D) is provably not concentrated in a single value. Thresholds (on p) are also established for the existence of induced acyclic tournaments of size i which are sharp for i = i(n) ^ <x. Further, a polynomial time heuristic is analysed and it is shown that produces a solution whose size is at least $\log_r$ n + @(yTog_r n). All of these results also carry over (with some slight changes) to a related model which allows 2-cycles.

For the next problem, given a simple directed graph D = (V, A), let the size of the largest induced acyclic subgraph (dag) of D be denoted by mas(D). Let D G D(n,p) be a random instance as in the previous chapter. We obtain improved bounds on the range of concentration, upper and lower bounds of mas(D). Our main result is that mas(D) > [2 $\log_q$ np — Xj, where q = (1 — p)$^{-1}$, X = 1 if p > $n^{-1/3+e}$ (e > 0 is any constant), X = W/(ln q) if p > C/n, and C, W are suitably large constants. This improves the previously known lower bounds given by Spencer and Subramanian, where there is an O(lnln np/ ln q) term instead of X. We also obtain a slight improvement on the upper bound, using an upper bound on the number of acyclic orientations of an undirected graph. We also analyze a polynomial-time heuristic to find a large induced dag and show that it produces a solution whose size is at least $\log_q$ np + @(ydog_q np). Our results also carry over to the related model D_2(n,p).

The next problem deals with random undirected graphs. We study the concentration of the largest induced paths, trees and cycles (holes) in the random graph model G (n,p), and prove a 2-point concentration for the size of the largest induced path and hole, for all p > $n^{-1/2}$ $\ln^2$ n. As a corollary, we obtain an improvement over a result of Erdos and Palka concerning the size of the largest induced tree in a random graph.

In the last problem, we consider the independence number of K_r-free graphs and linear k-uniform hypergraphs in terms of the degree sequence, and obtain new lower bounds for them. This answers some old questions raised by Caro and Tuza. Our proof technique is an extension of a method of Caro and Wei, and we also give a new short proof of the main result of using this approach. As byproducts, we also obtain some non-trivial identities involving binomial coefficients, which may be of independent interest.

Publications

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Abstract

Safe management of radioactive waste with minimum impact to environment is emerging as one of the major challenges in separation science. Advances in macromolecular chemistry such as invention of dendritic polymers (dendrimers) are providing unprecedented opportunities to develop effective separation processes for treatment of aqueous waste. Dendrimer macromolecules are a new class of polymeric material with tree-like architecture having unique properties such as high degree of branching unit, high density of surface functional groups and narrow molecular weight distribution. Size, shape and reactivity of dendrimers are determined by their generation and chemical composition. Studies on removal of radionuclides from aqueous waste have been carried out by the following four indigenously synthesized compounds; (i) Poly(amido)amine (PAMAM) dendrimer chelating agent by Dendrimer Assisted Ultrafiltration (DAUF), (ii) PAMAM dendron grafted-styrene divinylbenzene (PAMAM-SDB) chelating resin by adsorption, (iii) Diglycolamic acid functionalized-PAMAM dendron- styrene divinylbenzene (DGA-PAMAM-SDB) chelating resin in both aqueous and nitric acid medium by adsorption and (iv) Xanthate functionalized PAMAM dendrimer (XFPD) by precipitation.

Studies on ultrafiltration of U(VI) and Th(IV) through regenerated cellulose acetate membrane reveal that about 76-97% of U(VI) and Th(IV) are removed at pH 5-7. Removal of U(VI) and Th(IV) is due to adsorption/mass deposition of hydrolyzed actinide species on the membrane surface. The water soluble PAMAM dendrimer chelating ligand has shown greater ability to bind with U(VI) and Th(IV) metal ions. PAMAM dendrimer assisted ultrafiltration is effective in selectively concentrating the actinides in the retentate at weakly acidic to neutral medium. Studies on the adsorption of U(VI) and Th(IV) on $PAMAMG_3$-SDB chelating resin reveals that adsorption capacity of $PAMAMG_3$-SDB is dependent on contact time, pH, initial concentration of U(VI) and Th(IV) and

temperature. High decontamination factors were achieved for actinides by solid-phase adsorption using PAMAM-SDB chelating resin. Kinetic study shows that the adsorption process is fast and equilibrium is reached within 60 minutes. Adsorption follows pseudo-second order kinetics and Langmuir isotherm model suggesting chemical adsorption. Adsorption capacity of the chelating resin increases exponentially with increase in dendron generation. $PAMAMG_5$-SDB has adsorption capacity (q_e) of 493 and 261.5 mg g^{-1} for U(VI) and Th(IV) respectively. DGA-PAMAM-SDB chaleting resin is effective in removal of U(VI) and Th(IV) from both aqueous and nitric acidic medium. The adsorption capacity of DGA-$PAMAMG_5$-SDB for U(VI) and Th(IV) are 682 and 544 mg g^{-1} respectively. PAMAM dendrimer and dendron grafted-SDB chelating resins could be regenerated at acidic pH (< 2) and reusable. Xanthate Functionalized PAMAM Dendrimer (XFPD) ligand removes various metal ions from aqueous solution by precipitation at pH > 4. Actinides (U & Th) are precipitated as metal hydroxides along with other metal ions during the xanthate precipitation. Studies with radioactive liquid waste (RLW) show that percentage removal of radionuclides are in the following order; Zr(IV) ~ Eu(m) ~ Co(II) (> 99.8) > Ce(III) (98.84) > Sb(III) (83.31) > Ru(III) (79.44) > Mn(II) (54.29) > Cs(I) (24.02). Hence, XFPD ligand possesses potential applications in total decontamination of radioactive wastes. The overall objective of the research described here is to develop dendrimer based chelating agents for treatment of radioactive waste streams in nuclear facilities. The potential applications of dendrimer based chelating agents for removal of actinides and other radionuclides from aqueous medium are demonstrated in the thesis.

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Abstract

The thesis described the development of economical and environment friendly organosilicon precursors and deposition of different morphological SiC on graphite, zircaloy and carbon composite using different techniques to make composite materials suitable for use in nuclear industry and other purposes.

The thesis is divided into six chapters. Chapter 1, described the relevant literature survey to screen out non toxic, non corrosive and economical SiC precursors and different deposition techniques for SiC deposition on various materials including carbon and other surfaces. Chapter 2 deals with the synthesis of potential precursors of SiC. The molecular precursors such as 2,4,6-trimethyl-2,4,6-trisila-heptane, 2,4,6-trisilacyclohexane and a mixture of organosilicon compounds (named as CVDP) were synthesized for CVD application. The process parameters were optimized for bulk synthesis of CVDP precursor. In Chapter 3, coating studies were carried out on nuclear important materials such as graphite / zircaloy substrate using synthesized CVDP precursor and commercial available Hexamethyldisilane (HMDS). Both precursors yielded dense SiC coating on graphite and zirconia substrate at low deposition temperature. The comparative SiC deposition study on TRISO particles using commercial available precursors Methyltrichlorosilane (MTS), HMDS and Tetramethylsilane (TMS) have shown that the non toxic and non corrosive precursor HMDS can replace the corrosive and toxic MTS precursor. Further Taguchi method has been used to optimize the parameters in CVD process for growth of SiC nanowires. Chapter 4 deals with different sol-gel process for deriving SiC. Two step sol gel process was used for generating SiC material using tetraethylorthosilicate and phenol formaldehyde resin. A fabrication process has been developed to prepare SiC nanowire embedded-dense SiC matrix/carbon fiber composite. Chapter 5 comprised of the studies on thermal degradation behavior and kinetic of thermal decomposition of dense and nanowires morphology coated carbon samples and SiC impregnated carbon composites. Chapter 6 summarized the thesis and future outlook of the present investigation.

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Abstract

This thesis deals with mathematical objects known as planar algebras. These were introduced by Vaughan Jones in order to study the so-called 'standard invariant' of a I^-subfactor and have provided a powerful pictorial viewpoint with which to approach various computations in the theory.

Planar algebras are, at their simplest, a collection of vector spaces along with a (large) family of maps between their tensor products. The maps are indexed by pictures in the plane called planar tangles and are postulated to be compatible with simple planar operations on the planar tangles.

A fundamental result of Jones in [5] may be considered as ensuring a plentiful supply of planar algebras. According to this result, every finite index II_1 subfactor N C M yields, in a natural way, a planar algebra P = P^{N-M}. This planar algebra satisfies several niceness conditions, such as, for instance, finite dimensionality of the vector spaces involved. Planar algebras arising from sub-factors are called subfactor planar algebras and have an intrinsic definition, independent of subfactors. It is these subfactor planar algebras that we will be interested in.

As in group theory, there is a notion of universal planar algebras akin to that of free groups and any planar algebra is a quotient of a universal planar algebra. A universal planar algebra is determined by just a set L (which is a graded set and referred to as a set of labels). By imposing relations on a universal planar algebra we may obtain an arbitrary planar algebra. Such a generator-relation approach to a particular planar algebra is called a skein theory for that planar algebra. We will use the term in this thesis only when both generators and relations are finite sets.

Among the subfactor planar algebras, the analytically trivial ones are said to be of finite depth. These planar algebras are determined completely by a finite amount of data. Nevertheless they are interesting enough to include several classes of well studied planar algebras such as those associated to finite groups and subgroups or to finite-dimensional Kac algebras, the Temperley-Lieb planar algebras, the ADE type planar algebras as well as some exotic planar algebras such as the Haagerup and extended Haagerup planar algebras.

In each of these planar algebras, there has been work done to show that they have an interesting skein theory. Some of the papers dealing with skein theories include [9] for group subfactors, [6] for Kac algebra subfactors, [3] for higher exchange relation planar algebras, [1] for the ADE planar algebras and [10] and [2] for the Haagerup type planar algebras. In all these papers, one of the main points is an explicit construction of a skein theory for the planar algebras being considered.

In this thesis, we prove two results that are suggested by the previous work. These appear in Chapters 2 and 3 after a preliminary introduction to planar algebras in Chapter 1. A detailed summary of Chapters 2 and 3 follows.

The main theorem of Chapter 2 asserts that a finite depth planar algebra admits a skein theory, i.e., a presentation with finitely many generators and finitely many relations. Thus finite depth planar algebras constitute a subclass of analogues of finitely presented groups.

The first section is devoted to showing that for an arbitrary planar algebra P satisfying an analogue of the finite depth condition for subfactor algebras, there is a P_{k-1}-P_{k-1} bimodule

isomorphism P_m C_{Pfc_1} P_n ^ P_m+n-(k-1) for all m, n > k where k is the 'depth' of P.

The next section introduces the technical tools that we use to prove our main result. These are the notions of templates and consequences. A template is simply an ordered pair of planar tangles and thus is not a planar algebra dependent object. However, given any planar algebra P together with a subset B of P, there is a notion of a template being satisfied in (P, B). Consequences of a set of templates roughly correspond to closing this set under certain planar operations. It is not hard to see from the definitons that if certain templates are satisfied for (P,B), then so are all their consequences. The main result in this section is a collection of various consequences of a set of templates that we call basic templates.

The third section of this chapter proves our main theorem that subfactor planar algebras of finite depth have a finite skein theory. The approach is to show that the basic templates hold for such a planar algebra (together with the distinguished subset being a basis of Pk where k is the depth) and then use their consequences and the bimodule isomorphism referred to above to deduce the theorem.

The last section gives a very simple proof that finite depth subfactor planar algebras are actually singly generated and further have a skein theory with this single generator. This last result is analogous to a finitely presented group having a finitely generated kernel for any surjective homomorphism of a finitely generated free group onto it, and the proof is also an imitation of that proof.

The main problem that we deal with in Chapter 3 takes off from the single generation result proved in Chapter 2. If P is a subfactor planar algebra of depth k, then it is easily seen that it is singly generated by an element of P_{2k}.
However the number 2k is not the best possible and while we do not settle what is the best, we show that if 2t is the even number of k + 3 and k + 4, then min{2k, 2t} will do. This is, of course, better in case k > 4.

Much of the effort in reducing the bound on the degree of the generator is spent in proving a result about finite dimensional complex semisimple algebras that might be of independent interest. In the first section of this chapter, we show that if S is an anti-automorphism of such an algebra without an $M_2(C)$ summand, then there exists an element a in it such that a and Sa generate it as an algebra. The restriction about not having an $M_2(C)$ summand is necessary. The proof of this result exploits a factorization theorem due to Takagi [4] and some simple considerations about the Zariski topology.

The second section proves the bound asserted. This is a consequence of a graph theoretic lemma applied to the principal graph of the subfactor planar algebra along with the generation result of the earlier section.

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Abstract

Room temperature ionic liquids (RTILs) have come up as a class of novel compounds primarily because of their interesting physicochemical properties like very low vapour pressure, wide liquid range, moderate to high viscosity, high ionic conductivity etc. However, molecular-level understanding on the intermolecular interactions, structure, and dynamics of new solvent systems are very much essential so that these substances can be used to their full potential. The main objective of the present thesis is to understand the kinship among the structures, intermolecular interactions and dynamics in ionic liquids. A brief introduction on RTILs and outcome of the previous literature reports of studies on solute rotation and solvation dynamics in RTILs are presented in the first chapter of the thesis. In the second chapter, details of instrumental techniques and data analysis have been presented. The third and fourth chapters delineate the effect of solute-solvent interaction, ionic constituents on solvation[1, 2] and rotational dynamics[3, 4] of solute probes. The last two chapters (fifth and sixth) discuss in detail the effect of cosolvents on solute rotation and solvation dynamics[5, 6] and heterogeneity of RTILs[7, 8]. The future prospect and challenges are outlined at the end of the last chapter.

Publications

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Title	:	Optical Polarimetric Spectroscopy of Biological Systems

Abstract

In the thesis we have addressed some of the issues which can help enhance the utilization of spectral Mueller matrix polarimetry for applications in biomedical imaging and diagnosis. One of the important problems addressed by us is the measurement of Mueller matrix in backscattering geometry with same set of polarization optics in PSA and PSG. In this geometry a complete set of polarizer-analyser combinations cannot be generated with conventionally used polarization optics. We showed that by incorporating a Faraday rotator, a non-reciprocal polarization device, a complete set of polarization analyser states can be generated. This geometry will facilitate combining Mueller matrix measurements with optical coherence tomography or confocal microscopy to improve the information content in these imaging techniques.

Another important outcome of the thesis is the development of mathematical methods for characterizing the polarization parameters from partial Mueller matrix measurement performed using linear polarization measurements alone. This development avoids the need for wave-plates and thus allows a much larger spectral coverage. In addition a reduction in the required number of components and intensity measurements make the system simpler. We showed that under the assumption that the depolarization of incident light with linear polarization is independent of the orientation of linear polarization the partial Mueller matrix can be decomposed to obtain polarization parameters such as linear retardance, diattenuation and depolarization. We also showed that for non-depolarizing samples the incomplete Mueller matrix measurement performed using 9 linear polarization measurements, can be converted in to the 4><4 Mueller matrix. Therefore, the polar decomposition algorithms developed for the complete Mueller matrix can be used for determination of the polarization parameters (retardance and diattenuation) of a non-depolarizing medium.

Studies were also carried out on the use of depolarization properties of turbid medium for obtaining useful optical parameters. Our experiments showed that while for turbid medium containing Rayleigh scatterers, an increase in absorption leads to an expected decrease in depolarization due to truncation of long path photons, for large size scatterers, an increase in depolarization with an increase in absorption was observed. This was explained to be arising due to the fact that an increase in absorption causes a decrease in the fraction of multiply scattered

photons thereby increasing the contribution of the single scattered photons in the backscattcred light. For large sized scatterers the polarization of scattered light varies significantly with angle and would lead to depolarization when averaged over finite angle. Therefore an increase in the contribution of single scattered photons to backscattered light leads to an increase in the depolarization. Further we showed that depolarization map, which can be constructed by plotting depolarization for different elliptically polarized light Stokes vectors, shows significant scatterer size dependence while showing no significant absorption dependence.

Our studies on different gold nanoparticles showed that for all the shapes investigated the depolarization for circularly polarized light is a factor of two larger than that for linearly polarized input light. The results also suggest that the use of rod shaped particles and circularly polarized input light will lead to best depolarization contrast. Further, our results indicate that the use of depolarization contrast could be useful in imaging techniques such as polarization sensitive optical coherence tomography and in confocal microscopy, for which the multiple scattering contribution is small.

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3. “Backscattering Mueller matrix measurement scheme using the same polarizing- analyzing optics”, M. K. Swami, H. S. Patel, and P. K. Gupta, Journal of Optics, 2013 , 15, 035709 1-6.
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Title	:	Existence of Darboux Chart on some Frechet Manifolds

Abstract

Let (M, ω) be a finite dimension symplectic manifold with symplectic formω. The loop space $LM := C^{\infty}(S^1, M)$ is a nuclear Fr´echet manifold modeled onLR^{2n}. For$\gamma \epsilon LM$and $X, Y \in T_{\gamma} LM$,define $\Omega_{\gamma}^{\omega}(X, Y) = \int_0^1 \omega_{\gamma(t)}(X(\gamma(t), Y(\gamma(t))dt$.

$\Omega_{\gamma}^{\omega}$is a weak symplectic structure on the loop space. We proved that the loop space admits a Darboux chart for any ω. As a corollary of existence of Darboux chart, we showed that the symplectic cohomology of the loop space is equal to the de-Rham cohomology of loop space. Further we proved that the almost complex structure on LM compatible with $\Omega_{\gamma}^{\omega}$is weak integrable in local sense.

Next we move to a general class of a Frechet manifold known as PLB (ProjectiveLimit of Banach) manifolds. We define a notion of a compatible symplectic structure on the PLB manifolds. We associate to each point $x \in M$, a Frechet space Hx. We prove that if $Hx$are locally isomorphic, then with certain smoothness and boundedness condition, there exists aDarboux chart for the weak symplectic structure.

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Title	:	Interface Characterization of Multilayer Mirrors

Abstract

Thrust of this thesis is centered on development of short period grazing incidence hard x-ray mirrors and soft x-ray normal incidence mirrors with an aim that they can be used in Indus-1 and Indus-2 beamlines. Thesis focuses on development of preparation and analysis facilities for thin films and multilayers. To reach this objective moderate resolution reflectometer capable of carrying out x-ray reflectivity, grazing incidence diffraction and powder diffraction has been developed. Also, development of Ion Beam Sputtering based thin film deposition system has been carried out. These developed instruments were used for systematic analysis of W/Si, W/B4C and NbC/Si multilayers as function of thickness and multilayer period. The main achievement of this work is the identification of the minimum bilayer thickness which does not show intermixing across the internal interfaces during or after preparation. This information was revealed by systematic investigation of surface and interface of large number of single layer, bilayer and multiayer structures using x-ray reflectivity data and made the conclusion by comparing the determined parameters as function of the as-grown structure parameters. A second achievement

is the investigation of short period multilayers as function of annealing temperature. It is found out that the combination NbC/Si shows much higher thermal stability (up to 700°C) compared to Mo/Si multilayers which has similar reflectivity at room temperature in VUV spectral range.

Thesis has focused its investigation on the main reasons for interface degradation as function of film thickness. It has been established that the process of interaction of back reflected sputter gas atoms/ions with the deposited material is the most important reason for interface degradation at shorter periods. It has been confirmed by means of STRIM calculation that a measureable number of such ions/atoms can reach high energy and can release freshly deposited host atoms from the surface. These results are very important and have not been described in literature before.

Thesis also covers surface and interface studies carried out on NiMnSb thin films, Nb thin films, and Co/Si bilayers and multilayers. These studies were carried out to understand the structure and to relate the physical properties with the structure.

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Title	:	Equation of State and Electrical Conductivity of Materials

Abstract

In this chapter we report results of ab-initio calculations for the zerotemperatureisotherm for Al in compressed states. Zero-pressure properties, phase stability and phase coexistence have been studied for Al. Possible high pressure phases of Al are examined by comparing the total internal energies and enthalpies for three structures, viz., FCC, BCC and HCP. The energies are calculated using the density function formalism and the FP-LAPW method. Perdew-Burke- Ernzerhof 96 parametrization of the Generalized Gradient Approximation (GGA) is used for exchange and correlation. Zero pressure lattice constants and the bulk modulus have been calculated for three phases of Al, and show good agreement with published experimental results. Our results for the minimum energy c/a ratio for hcp match well with the experimental value. Coexistence of FCC & HCP phases for a wide range of pressures near phase transformation is indicated by volume energy curves, in agreement with a recently reported powder X-ray diffraction experiment. The calculated lattice parameters at high pressures show good

Publications

Journals

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3. A Comparison of Quotidian EOS of Al with Ab Initio Calculations, V. Mishra, Sijoy C.D., P. Pahari and S. Chaturvedi, Journal of Physics: Conference Series 377 (2012) 012105 (1-5)
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3. A Comparison of Quotidian EOS of Al with Ab Initio Calculations, V. Mishra, Sijoy C.D., P. Pahari and S. Chaturvedi, presented in International Conference on High Pressure Science and Technology, AIRAPT-23, BARC, Mumbai, 25-30 Sept, 2011.
4. EOS and Conductivity of Expanded States of Aluminium, V. Mishra V. Mehra and S. Chaturvedi, presented in International Conference on High Pressure Science and Technology, AIRAPT-23, BARC, Mumbai, 25-30 Sept, 2011.
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7. Computer Modelling of Electric Gun Aaditya V. Majalee, V. R. Ikkurthi, P. Pahari, V. Mishra, S. Chaturvedi, presented in International Conference on High Pressure Science and Technology, AIRAPT-23, BARC, Mumbai, 25-30 Sept, 2011.
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9. Chatturvedi, presented and published in the Proc. of Indo - Russian Workshop on High Energy density Physics for Innovative Technologies & Industry Applications, I2IT Pune , 19-21 Nov 2008.
10. Production of Megabar Pressure in Metallic Liner: A Computational Study S. Madhavan, V. Mishra, A. Majalee, P. Pahari and S. Chaturvedi, presented and published in the Proc. 52nd DAE Solid State Physics Symposium, University of Mysore, 27-31 Dec. 2007.

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Title	:	Estimation of Reactor Power from Core Temperature Signals

Abstract

1. Context

Nuclear reactors must follow stringent norms for their reliable and safe operation. To meet such requirements, all safety critical systems in Nuclear Power Plants (NPPs) must be validated using diverse methods. Presently in NPPs, measurement of generated thermal power is performed through neutronic channels, which also require validation. The neutronic readings are calibrated using absolute/steady state value of the core temperature at regular time intervals. Hence, there is a need for a diverse method to complement the existing power measurement. Also, presence of alternative method may help in facing complex and unforeseen situations such as unavailability of other monitoring systems. Hence, a new method for power measurement must be investigated to meet safety requirements.

2. Objectives

(i) To investigate the feasibility of using temperature fluctuations in coolant at the outlet of subassemblies to estimate reactor power.

(ii) To study the properties of associated temperature fluctuations at various reactor thermal power levels.

(iii) To propose a method to derive generated thermal power information from temperature fluctuations.

(iv) To estimate the resource utilization for a signal processing implementationon a FPGA-based reference platform.

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Title	:	Experimental and Data Modeling Methods for Targeted Water Chemistry Studies Related with Nuclear Power Reactors

Abstract

Water chemistry studies related to the decontamination of stainless steel based nuclear reactors and also application of ion exchange resins for maintaining the specific water chemistry has been carried out. Optimization of parameters for synthesis of vanadium in low oxidation state has been undertaken. Vanadium (II) compounds are suitable for reductive dissolution of oxide materials formed on stainless steel. Various solution conditions as well as different electrodes have been evaluated to synthesise V(II) optimally. Carbon based electrodes have been shown as better cathode material for electrolytic preparation of V(II). Solubility of V(V) and V(IV) in aqueous formic acid media has been evaluated to optimize the precursor solution concentration for electrolysis. The maximum aqueous solubility of V(IV) formate has been found to be more than that of V(V) formate. Controlled current electroreduction of these compounds at concentrations around 125 mM has resulted in formation of soluble V(II) formate in the medium while at higher concentrations, V(III) formate precipitated out upon electrolysis. Reduction of

V(IV) formate at 350 mM concentration using zing amalgam resulted in precipitation of V(II) formate. The chemical formulae of the vanadium compounds precipitated out by exceeding their solubility limits in the different oxidation states viz. V(V), V(IV), V(III) and V(II) were determined by a combination of chemical analysis, spectroscopic techniques, thermogravimetry, XPS and XRD. The formulae of the synthesized compounds were found to be V2O5, VO(HCOO)2-H2O, V(OH)(HCOO)2 and V(HCOO)2-2H2O respectively.

Methodology for redox speciation of aqueous vanadium solutions has been evolved. As vanadium (II) and Vanadium (III) are air-sensitive, inert atmosphere has to be maintained during the preparation. This is based on continuous solution potential monitoring with a redox electrode impressed with a high frequency alternating voltage to overcome polarization of the electrode. The redox speciation method for periodic batch samples has also been evolved which is based on simple, rapid and sensitive indirect spectrophotometric measurement. The samples were first converted into a V(V)/V(IV) mixture by adding excess V(V). V(V) in solution was then evaluated by adding Fe(II) and estimating the Fe(III) formed by the spectrophotometric determination of the sulfosalicylic acid complex where neither V(IV) nor Mn(II) has shown any interference over a wide range of concentration.

Chromate reduction on magnetite in presence of gamma irradiation has also been studied. The chromate reduction with dose follows a Lagergren's pseudo first order kinetic model. This process was found to be a surface phenomenon. The effect of reducing radiolytic species on both chromate solution and dispersed magnetite could be ascertained. XPS data for magnetite equilibrated with chromate under γ irradiation has shown a different surface composition as compared to the one obtained in absence of γ irradiation.

Nitric acid leachout characteristics from weak base anion exchanger has been experimentally evaluated as a function of total nitric acid loading at a given flow velocity. An empirical first order model is used to explain the column outlet behaviour. Based on the experimental evaluation, a column configuration of a strong acid cation exchanger topped mixed bed of strong acid cation exchanger and weak base anion exchanger followed by a 5% nitric acid loaded weak base anion exchanger as a bottom layer has been used to remove $Gd(NO_3)_3$ from water while maintaining the column outlet pH in the range of 5.0 - 5.5 which conforms to the technical specifications for moderator system during gadolinium removal.

Publications

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7-12 Dec., 2010, Mumbai, Poster paper No. A-23.\

3. "Electrochemical Synthesis and Characterization of $V(OH)(HCOO)_2$ for Easing the Decontamination Formulation Preparation Methodology for Light Water Reactors" V. S. TRIPATHI, K. K. Bairwa and S. Velmurugan, Proc. of Fifth ISEAC Triennial International Conference on Advances and Recent Trends in Electrochemistry (ELAC-2013), 16-20 Jan., 2013, Hyderabad, pp 485-489.

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Title	:	Role of Notch in Regulation of Gamma Delta T Lymphocytes and Regulatory T Cell Functions

Abstract

Integration of myriad signals is required for the activation of T cells. Among these, the Notch signaling pathway facilitates short range communication between cells. Indeed, transmission of Notch signals requires physical contact between cells under most circumstances. It is becoming increasingly clear that Notch signaling regulates peripheral CD4+, CD8+, Tregs and NK cells responses. In the present study, we evaluated the role of Notch in regulation of peripheral γδ (gamma delta) T cells and regulatory T cell functions.

We describe for the first time, to our knowledge, the role of Notch in regulating the effector functions of human γδ T cells. γδ T cells are involved in combating infectious diseases and have non-redundant capacities in the inhibition of tumor development and progression. The present study showed Notch1 and Notch2 expression in γδ T cells derived from healthy individuals and oral cancer patients at both mRNA and protein levels. Inhibiting Notch signaling in phosphoantigen/anti CD3mAb-stimulated γδ T cells resulted in marked decrease in proliferation of γδ T cells, confirming TCR engagement as a key initiating event. It was also observed that blocking of Notch signaling in γδ T cells by GSI-X as well specific silencing of either Notch1 or Notch2 by siRNA inhibits the ability of γδ T cells to lyse tumor targets. Similarly, obstructing Notch signaling inhibited the IFN-γ secretion by γδ T cells stimulated with phosphoantigens/anti CD3 mAb. These results showed that Notch signaling pathway plays an important role in regulating effector functions of γδ T cells. Furthermore, it was found that rDll1 and rDll41 augments whereas rJag1 significantly decreases phosphoantigens driven proliferation of γδ T cells. Similarly, rJag1 significantly decreases IFN-γ secretion by phosphoantigen/anti CD3 activated γδ T cells. Interestingly, we also found that blocking of Jag1 ligand on regulatory reduces their suppressive potential against γδ T cells. These studies may have important implications in clinical situations where new strategies for the clinical manipulation of γδ T cells for cancer immunotherapy are being investigated.

Publications

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Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	NN-Dialkylamides as Alternative Extractants in Nuclear Fuel Reprocessing

Abstract

Tri-w-butyl phosphate (TBP) dissolved in w-dodecane, has been used as workhorse in nuclear fuel reprocessing industry for the last five to six decades, yet a few drawbacks associated with it. Based on pioneering work of Siddall, N,N-dialkyl amides have been identified as alternative extractants of TBP due to their completely incinerable nature. N,N- dihexyloctanamide (DHOA) has been identified as a promising alternate to TBP in spent nuclear fuel reprocessing of Pressurized Heavy Water Reactor (PHWR).

The present research work deals with evaluation of DHOA vis-a-vis TBP as extractants for the reprocessing of fast reactor and Advanced Heavy Water Reactor (AHWR) spent fuels. Extraction data have been generated by batch experiments as well as by mixer settler/centrifugal contactors under the relevant conditions of fast reactors and AHWR fuels, respectively. A process flow sheet has been developed for the reprocessing of AHWR spent fuels under simulated conditions. DHOA shows better extraction ability for Pu and extraction of U is comparable to TBP. DHOA shows better stripping behaviour for U, Pu and Np as compared to TBP. Radiolytic and thermal degradation studies proved that DHOA is a promising alternative of TBP for spent fuel reprocessing. Np extraction studies and conditions for co-recovery of U, Pu and Np have been optimized using 1.1M TBP and 1.1M DHOA dissolved in w-dodecane as solvents under PHWR-HLW conditions. Tc extraction behavior was studied using DHOA and TBP solutions in w-dodecane, under varying experimental conditions. The experimental results suggested that 1.1 M DHOA is better than 1.1 M TBP with respect to co-extraction of Tc and U, and U decontamination with respect to Np/Pu.

Dynamic Light Scattering (DLS) studies were also carried out to investigate the aggregation behavior of 1.1 M solutions of TBP and DHOA. A significant enhancement in the aggregate sizes was observed with increasing concentration of thorium in the organic phase. The effect of uranium extraction on third-phase formation behavior was also studied using 1.1 M TBP and 1.1M DHOA solutions in different diluents viz. w-dodecane, 10% 1-octanol + w- dodecane, and decahydronaphthalene (decalin). An empirical correlation was developed for predicting the concentrations of uranium and thorium in HOP for both the extractants. Thermal decomposition studies of DHOA/w-dodecane system were carried out to explore the possible runaway reaction and red-oil formation in nitric acid medium.

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Title	:	Effect of a Methylxanthine Compound and Anticancer Agent on Integrin Mediated Adhesion and Induced Apoptosis in Breast Cancer Cells

Abstract

Triple Negative Breast Cancers (TNBC) raises an urgent need to develop an effective treatment since targeted therapies fail to combat the same. In this context, drug repurposing a process of ascertaining newer roles of existing drugs had been demonstrated. PTX, a methylxanthine derivative is an FDA approved drug for the treatment of peripheral vascular diseases. The project unravels the anti-metastatic effects of Pentoxifylline (PTX) in human MDA-MB-231 breast cancer cells. PTX affects the processes of cellular proliferation, adhesion, invasion, migration, apoptosis and angiogenesis. The process of adhesion to Extracellular Matrix (ECM) is in part mediated by cellular receptors such as the integrins. Loss of this adhesion mediates cellular death. PTX affects cellular adhesion to ECM components and its allied receptors integrins. The integrins lack the enzymatic activity and thus need accessory molecules such as Focal adhesion kinase (FAK) to mediate its downstream effect. Thus, effect of PTX was evaluated on FAK and its downstream effectors such as MAPK/ERK and Akt pathways, PTX affected active levels of MAPK and Akt, affecting cellular proliferation and culminating into cellular death or apoptosis. The effect of PTX was also ascertained on certain anti-apoptotic proteins such as Bel-2 family members and

caspases. PTX also affects cellular migration by affecting the actin cytoskeleton and activity of RhoGTPases. Finally, PTX causes a delay in tumor growth and affects the process of angiogenesis using in vivo model system. PTX along with liposomal doxorubicin also causes tumor growth delay. These investigations surely underlie the potential of PTX in the management of breast cancer

Publicatilons

Journal

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Title	:	Stability and Embedding Properties of Some Projective Manifolds

Abstract

My thesis is divided into two parts.

In the first part, we prove the semistability of logarithmic de Rham sheaves on log conical pair, under suitable conditions. This is related to existence of Kahler-Einstein metric on the open variety. We investigate this problem when the Picard number of smooth projective variety is one. We prove semistability of the logarithmic de Rham sheaf on log canonical pair under suitable hypothesis on the divisor components . We also extend the semistability result for Kawamata coverings, and this gives examples whose Picard number can be greater than one. Finally, we proved semistability of log Fano manifolds of dimension at most 6.

In the second part, we investigate linear systems on hyperelliptic varieties. We prove analogues of well-known theorems on abelian varieties, like Lefschetz's embedding theorem and higher higher jet embedding theorems on hyperelliptic varieties. Syzygy properties are also deduced for appropriate powers of ample line bundles on hyperelliptic varieties.

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2. S. Chintapalli, J. N. Iyer : Embedding Theorems on Hyperelliptic Varieties . Geom. Dedicat a , 171:249-264,2014

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Title	:	Experimental and Computational Investigation of H2-F2 Reaction in a Tubular Reactor

Abstract

The reported work addresses the important problem of change in the behaviour of the H_2- F_2 flame reactor under the influence of various parameters such as, excess hydrogen, flow rates, preheating of the reactor wall, addition of different types of diluents etc., through experimental studies and computational modeling. An extensive review of the existing literature on H_2-O_2 and H_2-F_2 systems has been presented in the thesis. Meticulously planned experiments with adequate safety in design for H_2-F_2 handling and reaction have been carried out in two types of reactors; a vertical cylindrical reactor (VCR) for flow trials, and, a horizontal cylindrical reactor (HCR) for batch operations. The experiments conducted in the VCR have among other things, indicated the following: (1) the reaction takes place a little away from the feed nozzles, (2) the influence of excess hydrogen is limited to a distance of 120 mm from the tip of the fluorine feed nozzle, (3) the reactor wall temperature significantly affects the temperature profile of the reactor, and (4) the diluents such as helium, nitrogen and argon cause a significant decrease in the temperatures near the fluorine feed nozzle, thereby reducing the thermally induced fluid velocities. The temporal behaviour of gas temperatures inside the HCR are reasonably predicted by the analytical model. The CFD model has been developed using the commercial software, FLUENT, which allows to simulate the complex geometries while solving momentum, energy, species transport, reactions and turbulence in the computation of the flow experiments. Selection of k-s as the turbulence model and grid size of 1 mm have produced results which match well with the experimental temperature data. The radiative mode of heat transfer is found to be not so significant in the flame reactor. The validated CFD tool has been used for predicting the operating conditions of the scale-up designs of the reactor. Three scale-up designs of the H2-F2 flame reactor have been simulated and the results are reported in the work. Different criteria have been studied for the feed nozzle design and similar enthalpy per unit reactor volume has been considered as the basis for reactor sizing. The scale-up based on the similar velocities at the feeding nozzle exits has yielded better results but needed some improvisation in order to extend the higher temperature regime in the reactor. This to some extent is achieved by addition of nitrogen in the fluorine stream.

The work presented in the thesis is a good contribution to the development of an industrial scaleflame reactor which can serve as a model for several other similar applications, especially where the reactions are potentially dangerous because of possibility of explosions under uncontrolled conditions.

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Title	:	Investigations on High Power Solid State RF and Microwave Amplifiers for Superconducting Structures

Abstract

The radio frequency and microwave power amplifiers are key systems for superconducting accelerating structures. Major constituent blocks of a typical high power solid-state amplifier are power amplifier modules, power combiner, dividers and directional coupler. The objective of this research work is to explore newer design techniques and topologies suitable for high power and efficient operation of these constituent blocks, followed by their experimental verification.

For amplifier modules, the traditional and newer continuous operating modes are investigated for high power application. Unlike conventional designs at low power, the present analysis aims to explore a design space at high power, to operate the commercially available device, within its practical limits of drain voltage excursion. The traditional designs (Class A, B and AB modes) include two low power (10 W) and two high power (270 and 400 W) amplifiers. The newer designs include, two efficient variants of the Class J mode UHF amplifier in 500-700 W power regime, and an extended continuous Class F mode amplifier, capable of delivering 600 W. For power combiners, design of a novel multi-way radial topology is proposed. Using segmentation method, 8-way and 16-way combiners were physically demonstrated for their operation in kW level power range, having combining efficiency as good as 98.9%. For low power dividers, performance enhancement was achieved by its loading, separately with a capacitive stub and a dielectric-resonator. Similarly, for the directional couplers an improved design using asymmetrical and uniformly aperture coupled transmission line, is investigated. These constituent blocks, once integrated using a suitable architecture, yield kW level of power. In an effort to study such integrated system, an analysis is presented for the graceful degradation and amplitude/phase imbalance using a scattering parameter based model, followed by experimental investigation of 2 kW, 20 kW and 50 kW solid-state amplifier systems. This research work

provides useful design and experimental data for the high power radio frequency and microwave solid state amplifiers.

Publications

Journal

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Title	:	Trace Analysis of Lanthanides and Actinides Using Liquid Chromatography

Abstract

Separation and determination of lanthanides, thorium and uranium are of great significance in nuclear technology, environmental science, geochemistry, material science etc. Present thesis deals with the development of liquid chromatographic methods to suite the requirement of nuclear industry and environmental samples, where interferences from matrix elements is a perennial problem in addition to the challenges posed by the close similarities in the properties of the analyte elements. One of the objectives was to develop a method for the separation of lanthanides based on ion interaction chromatography. An ion interaction reagent, octadecyl sulphonate, which would offer high resolution separation and long term adsorption stability to

the stationary phase, was identified for the individual separation of lanthanides. Another LC method for the determination of lanthanide fission products was developed and this method does not involve any pre-separation of matrix elements. The direct method thus minimizes the chances of analyte loss or cross contamination during the sample preparation steps. In the present work, reversed phase chromatography was used for the separation of thorium and uranium as they form hydrophobic complexes with hydroxycarboxylic acid eluents. The unique elution pattern exhibited by mandelic acid eluent was explored for the development of a method for the determination of small amounts of uranium in thorium matrix. Studies were also carried out to unravel the reason behind this unusual elution order by employing different ion interaction reagents. Studies for the pre-concentration as well as analytical separation were carried out with an aim to determine uranium present at ultra-trace levels in seawater and processed seawater samples. In addition to good sensitivity and wide dynamic range, the developed method offers excellent tolerance to iron. Speciation studies of uranyl-hydroxycarboxylic acid systems were carried out using electrospray ionisation mass spectrometry to identify the species responsible for their adsorption/elution under chromatographic conditions. Influence of solution phase conditions as well as instrumental parameters on the distribution of major uranyl species was studied in detail to obtain sensitive and representative mass spectra. In nutshell, the thesis presents the work carried out to systematically study the effect of various chromatographic parameters to develop methodologies suiting specific samples and requirements.'

Publications

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1. Direct determination of lanthanides in simulated irradiated thoria fuels using reversed phase high-performance liquid chromatography P.G. Jaison, Narendra M. Raut, Suresh K. Aggarwal Journal of Chromatography A, 1122 (2006) 47-53.
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1. Determination of Uranium in Seawater by Liquid Chromatography Using Mandelic Acid as a Complexing Agent P.G. Jaison, V.M. Telmore, Pranaw Kumar and S.K. Aggarwal 34th International Symposium on High-Performance Liquid Phase Separations and Related Techniques (HPLC2009) held in Dresden, Germany during June 28 - July 2,2009, Paper No. ENV10, p. 324.
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8. Electrospay Ionization Mass Spectrometric Studies on Uranyl-Mandelic Acid Complex P.G. Jaison, Pranaw Kumar, V.M. Telmore, D. Alamelu and S.K. Aggarwal 12th ISMAS Triennial International Conference on Mass Spectrometry (12th ISMAS-TRICON-2013) held in Cidade-de-Goa, Dona Paula, Goa during March 3-8, 2013, Paper No. CP - 27, page 230.

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Title	:	A Journey towards QCD Radiative Corrections in the SM and Beyond at the LHC

Abstract

In this thesis, our main endeavor has been to pave the way towards next-to- leading order (NLO) QCD corrections for processes in the Standard model (SM) and beyond to the fullest extent. We mark off available standard techniques to perform NLO QCD corrections at the hadron collider and fit out a brief introductory portion on few beyond standard model scenarios in the first chapter. In the second chapter, we study the prospects of probing large extra dimension model at the Large Hadron Collider (LHC) through neutral triple gauge boson production processes. In theories with extra dimensions, these processes result from the exchange of a tower of massive graviton modes between the SM particles. We consider γγγ, γγZ, γZZ and ZZZ production processes and present our results for various kinematic distributions at the LHC with center of mass energy √S = 14 TeV. Also, we perform a detailed calculation of 5-point tensor integral reduction using Passarino-Veltman technique and present its analytical results in a ready-to-use format, so that they can be used whenever attempts to do NLO corrections of these processes are being made. The third chapter consists of NLO QCD corrections to the associated production of the vector boson (Z/W±) with the Kaluza–Klein modes of the graviton in the large extra dimension model at the LHC. We have obtained various kinematic distributions using a Monte Carlo code which is based on the two cutoff phase space slicing method that handles soft and collinear singularities appearing at the NLO level. We estimate the impact of the QCD corrections on total cross section as well as on various observables and find that they are significant. We also show the reduction in theroretical scale uncertainty when QCD corrections are included. Further, we discuss the ultraviolet sensitivity of the theoretical predictions. We present the NLO predictions for diphoton production in the ADD model in the fourth chapter. Fixed order NLO

results are matched to the HERWIG parton shower using the MC@NLO formalism. A selection of the results is presented for d = 2–6 extra dimensions to NLO+PS accuracy, using generic cuts as well as analysis cuts mimicking the search strategies as pursued by the ATLAS and CMS experiments. Finally, in the last chapter, we summerise our pivotal observations.

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8. G. Das, P. Mathews, V. Ravindran, and S. Seth, "RS resonance in di-final state production at the LHC to NLO+PS accuracy", Submitted in JHEP (2014) [arXiv:1408.3970].

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1. M. Kumar, P. Mathews, V. Ravindran, and S. Seth, "Associated Production of Vector Gauge Boson & Graviton to NLO QCD", PoS RADCOR2011 (2011) 047.
2. † M. Mandal, P. Mathews, V. Ravindran, and S. Seth, "Diphoton production in the ADD model to NLO+parton shower accuracy at the LHC", PoS RADCOR2013 (2013) 030
3. M. Mandal, P. Mathews, V. Ravindran, and S. Seth, "Tri-vector boson production at NLO with parton shower", PoS RADCOR2013 (2013) 035

Name	:	**Anil Kumar C.P.**
Enrolment No.	:	MATH10200804001
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Title	:	Orbits of Pairs in Finite Modules over Discrete Valuation Rings and Permutation Representations

Abstract

ABSTRACT. Let $\mathbb{A}$ be a discrete valuation ring whose maximal ideal is generated by a uniformizing element π, and which has a finite residue field $\mathbb{F}_q$. Let Λ denote the set of all sequences of symbols of the form

$$(\lambda_1^{\rho_1}, \lambda_2^{\rho_2}, \ldots, \lambda_k^{\rho_k}), \tag{1}$$

where $\lambda_1 > \lambda_2 > \ldots > \lambda_k$ is a strictly decreasing sequence of positive integers and $\rho_1, \rho_2, \ldots, \rho_k$ are positive integers. We allow the case where $k = 0$, resulting in the empty sequence, which we denote by $\emptyset$. Every finite $\mathbb{A}$-module $\mathcal{A}_{\underline{\lambda}}$ is, up to isomorphism, of the form

$$\mathcal{A}_{\underline{\lambda}} = (\mathbb{A}/\pi^{\lambda_1}\mathbb{A})^{\oplus\rho_1} \oplus (\mathbb{A}/\pi^{\lambda_2}\mathbb{A})^{\oplus\rho_2} \oplus \ldots \oplus (\mathbb{A}/\pi^{\lambda_k}\mathbb{A})^{\oplus\rho_k} \tag{2}$$

for a unique $\underline{\lambda} \in \Lambda$. Let $\mathcal{G}_{\underline{\lambda}}$ denote the automorphism group of $\mathcal{A}_{\underline{\lambda}}$.

Fix a $\underline{\lambda} \in \Lambda$, the corresponding finite torsion $\mathbb{A}$-module $\mathcal{A}_{\underline{\lambda}}$ and its automorphism group $\mathcal{G}_{\underline{\lambda}}$. The group $\mathcal{G}_{\underline{\lambda}}$ acts on ${\mathcal{A}_{\underline{\lambda}}}^n$ by the diagonal action

$$g \cdot (x_1, \ldots, x_n) = (g(x_1), \ldots, g(x_n)) \text{ for } x_i \in \mathcal{A}_{\underline{\lambda}} \text{ and } g \in \mathcal{G}_{\underline{\lambda}}.$$

In this thesis we study the set of $\mathcal{G}_{\underline{\lambda}}$-orbits in ${\mathcal{A}_{\underline{\lambda}}}^n$ under the above action for $n = 2$. We find that the cardinality of each orbit is a polynomial in q with integer coefficients and moreover, given such a polynomial, the number of orbits with that cardinality is a polynomial in q with integer coefficients which does not depend on $\mathbb{A}$, but only on the cardinality of the residue field of $\mathbb{A}$.

We use these results to analyze the permutation representation of $\mathcal{G}_{\underline{\lambda}}$ on the vector spaces $\mathbb{C}[\mathcal{O}]$ where $\mathcal{O}$ runs over $\mathcal{G}_{\underline{\lambda}}$-orbits in $\mathcal{A}_{\underline{\lambda}}$. We are able to prove that these permutation representations are multiplicity free.

Publications

1. Published: Title: On Fuglede's Conjecture For Three Intervals. Author(s): C.P. Anil Kumar, Bose D, Krishnan R, and Madan S. Journal: Online Journal of Analytic Combinatorics, No. 5. Art. 1, 24 pages, 2010.
2. Published: Title: Orbits of Pairs in Abelian Groups. Author(s): C.P. Anil Kumar, Amritanshu Prasad. Journal: Seminaire Lotharingien de Combinatoire, Vol. 70, Art. B70h 24 pages, 2014
3. Submitted: Title: Approximation of 4-sets by Rational 4-sets with Rational Area in the Plane. Author: C.P. Anil Kumar. Journal: International Journal of Number Theory.
4. Preprint (Second Part of My Thesis):itle: On some Multiplicity Free Permutation Representations of the Automorphism Group of a Finite Torsion Module over a Discrete Valuation Ring having finite Residue Field. Author: C.P. Anil Kumar.

Name	:	**Manju Taxak**
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Title	:	Interaction of Hydrogen with Tantalum Metal and its Alloys

Abstract

Tantalum is a potential candidate material for the hydrogen separation membrane due to its large hydrogen solubility and good hydrogen diffusivity. The permeability is a product of solubility and diffusivity. The hydrogen solubility in tantalum and its alloys is one of the parameters responsible to estimate the permeability. The hydrogen embrittlement associated with tantalum at low temperature is the main limitation of its use in membrane applications. Alloying with the elements which are having less hydrogen solubility or destabilize the hydrides can be a way to overcome this limitation. In the present work, the effect of nickel, chromium, iron and aluminium on the solubility of hydrogen in tantalum has been investigated. Ta-alloys with Ni, Cr, Fe and Al within solid solubility limit were prepared using arc melting in an inert atmosphere. Pressure- composition-isotherms (P-C-T) equilibrium measurements have been investigated in the temperature range (673-873) K for Ta-H and Ta-M-H systems [M = Ni, Cr, Fe and Al] using a Sievert's apparatus. The dissolved hydrogen was within the solid solubility range corresponding to the temperature and followed the Sievert's law. From the equilibrium P- C-T data, the thermodynamic parameters: the relative partial molar enthalpy, entropy and Gibb's free energy for the solution of hydrogen in these alloys are evaluated using Sievert's relationship. The hydrogen solubility in tantalum-alloys decreases with increase in the alloying elements composition. This decrease in solubility is attributed to increase in lattice strain energy of the alloys or due to very less solubility of hydrogen in these elements or the chemical inertness of these alloying elements towards the hydrogen. The relative partial molar enthalpy becomes less negative with increase in alloying elements composition whereas entropy values are almost constant.

In addition, the isothermal hydrogen absorption kinetics of unalloyed tantalum and tantalum-aluminium alloys has been investigated in the temperature range of (673973) K. The reacted fraction of hydrogen, a, was calculated from the experimental data of hydrogen absorption in different tantalum-aluminium alloys as a function of time using pressure drop method. The function g(a), giving the best linearity with time is indicative of the mechanism of hydrogen absorption. The rate function of hydrogen absorption and the kinetic parameters are obtained from the linear regression fitting of g(a) versus time plots. The mechanism of three-dimensional diffusion is the intrinsic rate-limiting step of hydrogen absorption processes in the studied temperature range. The apparent activation energy for the absorption of hydrogen in these alloys also calculated using Arrhenius equation that increases linearly with increase in the aluminium content in the alloys.

The thermodynamic and kinetics data for the solution of hydrogen in tantalum and its alloys can be used to process the design for Ta-based materials for various hydrogen atmosphere applications and can also be utilized in various modeling studies for hydrogen solubility and permeability.

Publications

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1. Manju Taxak, S. Kumar, S. Sheelvantra, N. Krishnamurthy, Effect of iron on the solubility of hydrogen in tantalum, Journal of Materials Science, Accepted. DOI: 10.1007/s10853-014 8557-9
2. Manju Taxak, Sanjay Kumar, N. Krishnamurthy, Thermodynamic Parameters for the Ta-Cr-H Solid Solution from Equilibrium P-C-T Data, J. Chem. Thermodynamics, 67 (2013) 48-54.
3. Manju Taxak, S. Kumar, B. Kalekar, N. Krishnamurthy, Effect of nickel addition on the solubility of hydrogen in tantalum, Int. J. Hydrogen Energy, 38 (2013) 7561-7568.

4. Manju Taxak, Sanjay Kumar, N. Krishnamurthy, A.K Suri, G.P.Tiwari, Change in lattice parameter of tantalum due to dissolves hydrogen, Int. J of Processing and Application of Ceramics, 6(2) (2012) 73-76.
5. Manju Taxak, N. Krishnamurthy, Effect of Aluminum on Hydrogen Absorption Kinetics of Tantalum, Journal of alloys and compounds. Revision required.
6. Manju Taxak, S. Kumar, N. Krishnamurthy, Thermodynamic Parameters for the Solubility of Hydrogen in Tantalum-Aluminium Alloys. To be communicated.

Conference Papers

1. Manju Taxak, S. Kumar, B. Kalekar, S. Smita, N. Krishnamurthy, "Effect of Aluminium on Hydrogen Solubility in Tantalum" Hydrogen and Fuel Cells Conference-2013. Accepted. Held in Napa Valley, California. July 12-15, 2013.
2. Manju Taxak, S. Kumar, S. Smita, B. Kalekar, N. Krishnamurthy, "The Effect of Iron on the Solubility Behavior of Hydrogen in Tantalum" Proceedings of 5th International Conference on Hydrogen Safety, Brussels, Belgium, September 9-11, 2013. ID: 100, P. 112.
3. Manju Taxak, S. Kumar, S. Smita and B. Kalekar, "Solid Solubility of Hydrogen in Ta-Cr Alloys" Proceedings of DAE-BRNS 4th Interdisciplinary Symposium on Materials Chemistry, Editors: D. Tyagi, A.M. Banerjee, K. Bhattacharyya, S. Nigam, S. Verma, A.K. Tripathi, D. Das, Mumbai, India 2012. P. 157-158.Manju Taxak, S. Kumar, B. Kalekar, S. Smita, N. Krishnamurthy, A K Suri and G.P Tiwari, Solid Solubility of Hydrogen in Ta-Ni alloys, Proceedings of National Symposium on Materials and Processing, Editors: A. Ghosh, A.K. Sahu, C.S. Vishwanadhan, S. Ramnathan, R.C. Hubli, G.P. Kothiyal, Mumbai, India 2012. P. 311-313.Manju Taxak, S. Kumar, A. Mukherjee, N. Krishnamurthy and A. K. Suri "Lattice expansion of tantalum due to dissolved hydrogen" Proceeding of the 18th International Symposium on Thermal Analysis, Editors: R. Agrawal, L Varshney, Y.K Bhardwaj, R.A Jat, S.K Rakshit, K.L Ramkumar, Mumbai, India 2012. P. 333-335.

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Title	:	Some Aspects of Gamma-Ray Astronomy

Abstract

This thesis focuses on some aspects of gamma-ray astronomy. The substantial part of this thesis deals with the experimental project in gamma-ray astronomy based on High Altitude GAmma Ray (HAGAR) telescope system which is located at an altitude of 4270 m in the Ladakh region of the Himalayas in India. Detailed Monte Carlo simulations pertaining to HAGAR system are carried out to determine the performance parameters of the system. Various performance parameters like energy threshold, effective area and detection rates have been estimated for vertically incident showers of different primaries (γ-ray, proton, helium, etc) as well as for inclined showers. We found that the energy threshold of the HAGAR telescope system is about 208 GeV, and it is able to detect Crab like sources at 5 sigma significance in $\sim$ 17 hours of observation. In addition, we have compared our simulated results with the observed results. The estimated trigger rate agrees well with the observed trigger rate of 13Hz. It has also been found that= the simulated trigger rates at various zenith angles are consistent with the corresponding observed trigger rates. We have observed the Crab nebula with the HAGAR telescope array. Regular source observations have begun with the complete setup of 7 telescopes since September 2008. The analysis of 10.4 hours (after data quality selection) of the Crab nebula data from the period 2008–2011 gives 5.6 ± 0.6 γ-rays/min with 8 σ significance. In addition, several Galactic sources such as LSI 61+303, MGRO J2019+37 are studied through the analysis of data taken with the HAGAR system.

The remaining part of this thesis is on phenomenological aspects of gamma-ray astronomy. In this context, two Galactic sources are studied through multi-wavelength modelling. The Milagro collaboration has recently reported an extended TeV gamma-ray source MGRO J2019+37 in the Cygnus region. No confirmed counterparts of this source are known although possible associations with several known sources have been suggested. We studied the spectral energy distribution (SED) of the source using a leptonic model for the TeV emission within the context of a Pulsar Wind Nebula (PWN), using constraints from multi-wavelength data from observations made on sources around MGRO J2019+37. These include a radio upper limit given by the Giant Meter wave Radio Telescope (GMRT), GeV observations by Fermi-LAT, EGRET and AGILE and VHE data taken from Milagro. We find that, within the PWN scenario, while leptonic model can explain the TeV flux from this source, the upper limit from the radio observation using GMRT imposes a stringent constraint on the size of the emission region.

Additionally, multi-wavelength modelling was done for another galactic source Cassiopeia A (Cas A). Non-thermal X-ray emission from the shell of Cas A has been an interesting subject of study, as it provides information about relativistic electrons and their acceleration mechanisms in the shocks. The Chandra X-ray observatory revealed the detailed spectral and spatial structure of this SNR in X-rays. The spectral analysis of Chandra X-ray data of Cas A shows unequal flux levels for different regions of the shell, which can be attributed to different magnetic fields in those regions. We have explained the GeV – TeV gamma-ray data in the context of both leptonic and hadronic scenario. We use the synchrotron emission process to explain the observed non-thermal X-ray fluxes from different regions of the shell. These result in estimation of the model parameters, which are then used to explain the TeV spectrum. We also use a hadronic scenario to explain both GeV and TeV fluxes simultaneously. We show that leptonic model alone cannot explain the GeV – TeV data. Therefore, we need to invoke a hadronic model to explain the observed GeV – TeV fluxes. We found that although a pure hadronic model is able to explain the GeV – TeV data, a mixed lepto-hadronic model provides the best fit to the data.

Publications

Journals

1. A study of the performance parameters of the High Altitude Gamma Ray (HAGAR) Telescope System at Ladakh in India Saha, L., Chitnis, V. R., Vishwanath, P. R., Kale, S., Shukla, A., Acharya, B. S., Anupama, G. C., Bhattacharjee, P., Britto, R. J., Prabhu, T. P., Singh, B. B. Astroparticle Physics, Volume 42, February 2013, Pages 33-40
2. Origin of gamma rays in the shell of Cassiopeia A Saha, L., Ergin, T., Majumdar, P., Bozkurt, M. & Ercan, N. Astronomy & Astrophysics, Volume 563, March 2014, A88

Conferences

1. TeV γ-ray source MGRO J2019+37 : PWN or SNR? Saha, L. & Bhattacharjee, P. In the proceedings of the International Astronomical Union, January 2013, Volume 9, 300-304, doi:10.1017/ S1743921313009629
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3. Monte Carlo simulation for High Altitude Gamma Ray Telescope System at Ladakh in India Saha, L., Acharya, B. S., Anupama, G. C., Britto, R. J., Bhattacharjee, P., Chitnis, V. R., Kale, S., Prabhu, T. P., Shukla, A., Singh, B. B., Vishwanath, P. R. In the proceedings of 32nd International Cosmic Ray Conference at Beijing, China, August 2011, Volume 9, 198-201

Others

1. Constraint on the pulsar wind nebula scenario of origin of the TeV gamma ray emission from MGRO J2019+37 in the Cygnus region Saha, L. & Bhattacharjee, P. Submitted to an International Journal.

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Title	:	Chromatographic and Mass Spectrometric Studies for Lanthanides, Actinides and Platinum Group Elements

Abstract

The Thesis entitled "Chromatographic and Mass Spectrometric Studies for Lanthanides, Actinides and Platinum Group Elements" by Mr. Pranaw Kumar consists of six Chapters. Chapter 1 describes the introduction of the Chromatography and Mass Spectrometry. In this regard the basic principles of these two techniques are explained. This Chapter also presents the literature survey of the existing methods for the separation of Lanthanides, Actinides and Platinum Group Elements and need for the development of the new methodologies.

Chapter 2 presents the importance and difficulties in the separation of the rare earths in bulk of the rare earth. Here, liquid chromatographic method was developed for the separation of lanthanides and yttrium from Dy_2O_3. Comparison of two reversed phase columns viz. Ci_8 and C_8 were carried out in order to enhance the resolution amongst the adjacent lanthanides. C_8 column using n-octane sulphonate as IIR provided better resolution and it was possible to resolve Y from Dy using a-hydroxyisobutyric acid (HIBA) as a single eluent.

Chapter 3 highlights HPLC based method for the separation of Lns, Th, U and Pu in the irradiated (Th, Pu)O_2 fuel. Two steps separation procedure was developed for the separation of lanthanides and actinides. A dynamically modified reversed phase column using n-octane sulfonic acid as an ion interaction reagent and dual gradient (pH and concentration) of HIBA were employed for separation of lanthanide fission products from the irradiated samples.

Chapter 4 describes the use of mandelic acid as an eluents for the separation of Th, U and Pu from the irradiated (Th, Pu)O_2 fuel. Using this method, U and Pu were eluted prior to the Th which prevents the interference from the Th.

Chapter 5 presents the usefulness of the electrospray ionization mass spectrometric studies for different species of platinum benzoylthiourea. Various species of platinum and benzoylthiourea were identified in positive and negative modes. The possible formation pathways were presented and the spatial arrangement predicted using density functional theory.

In Chapter 6, ESI-MS method was investigated for the determination of palladium in simulated high level liquid waste. Preconcentration of Pd-BTU complex was carried out selectively on disposable pipette containing C_{18} material. The suitability of the method was studied for determination of Pd in simulated high level liquid waste and there were no interferences from the neighboring elements namely Ag, Au, Cd, Rh and Ru.

Publications

1. Determination of Lanthanides and Yttrium in High Purity Dysprosium by RP- HPLC using a-Hydroxyisobutyric acid as an Eluent Pranaw Kumar, P.G. Jaison, D. R. M. Rao, V.M. Telmore, A. Sarkar and Suresh K. Aggarwal J. Liq. Chromatogr. Rel. Technol. 36 (2013)1513-1527.
2. Determination of Lanthanides, Thorium, Uranium and Plutonium in Irradiated (Th, Pu)O2 by Liquid Chromatography using a-HydroxyIsoButyric Acid (a-HIBA) Pranaw Kumar, P.G. Jaison, Vijay M. Telmore, Sumana Paul and Suresh K. Aggarwal Int. J. Anal. Mass Spectrom. Chromatogr. 1 (2013) 72-80.
3. HPLC Method for Determination of Th, U and Pu in Irradiated (Th,Pu)O2 using Mandelic Acid as an Eluent Pranaw Kumar, Sumana Paul, P. G. Jaison, Vijay M. Telmore, D. Alamelu, and

Suresh K. Aggarwal Radiochim Acta; DOI : 10.1515/ract-2013-2242

4. Speciation of platinum-benzoylthiourea in gas phase using electrospray ionization mass spectrometry and density functional theory Pranaw Kumar, P. G. Jaison, Mahesh Sundararajan, Vijay M. Telmore, Swapan K. Ghosh and Suresh K. Aggarwal Rapid Commun. Mass Spectrom. 27 (2013) 947-954.
5. Determination of Palladium by Electrospray Ionization Mass Spectrometry after Pre-concentration by Disposable Pipette Extraction P.G. Jaison, Pranaw Kumar, Vijay M. Telmore and Suresh K. Aggarwal Rapid Commun. Mass Spectrom 26 (2012) 1971-1979.

Symposia:

1. Investigations for Trace Determination of Gd, Tb and Ho in Presence of Large Amounts of Dysprosium by HPLC, Pranaw Kumar, P.G. Jaison, D. R. M. Rao, V.M. Telmore, A. Sarkar and S.K. Aggarwal, Nuclear and Radiochemistry Symposium (NUCAR) 2011, paper No. B-30, page No. 232.
2. Electrospray Ionisation Mass Spectrometry (ESI-MS) of Platinum-Benzyolthiourea (Pt- BTU) Pranaw Kumar, P.G. Jaison, V.M. Telmore and S.K. Aggarwal ISMAS International Discussion Meet on Elemental Mass Spectrometry in Health and Environmental Sciences (ISMAS-DM-HEAL-2011) during April 14-15, 2011in New Delhi, CP-5, Pg. 126.
3. Determination of Palladium by Electrospray Ionization Mass Spectrometry after Pre-concentration by Disposable Pipette Extraction P.G. Jaison, Pranaw Kumar, V.M. Telmore and S.K. Aggarwal 14th ISMAS Symposium cum Workshop on Mass Spectrometry (14th ISMAS-WS 2011) held in Munnar during November 7 - 11, 2011, CP - 33, p.223.
4. Studies on Species of Platinum (II) Complex with Benzyolthiourea in Acetonitrile Solution by Electrospray Ionization Mass Spectrometry Pranaw Kumar, P.G. Jaison V.M. Telmore and S.K.Aggarwal 14th ISMAS Symposium cum Workshop on Mass Spectrometry (14th ISMAS-WS 2011) held in Munnar during November 7 - 11, 2011, CP-32, p. 219

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Title	:	Lentiviral Vector Mediated Long Term Expression of Therapeutic Proteins

Abstract

Lentiviral vector (LV) mediated gene transfer has been put to varied uses and versatility of the system is continuously expanding. New vector platforms with expanded utility as well as its novel use for potential therapeutic benefits are also being investigated.

In the present study, the candidate has successfully delivered shRNA using LV against elastase in HEK-293. Increased production of rhEPO was found with this knock down strategy. Also the recombinant protein was purified and shown to have bioactivity. He has demonstrated the increased therapeutic potential of LV delivered cpp tagged murine interferon-α both in vitro and in vivo. Also the Galectin3 pseudotyped LV mediated targeted delivery and consequent antitumor therapeutic benefit was shown in vivo. He has effectively demonstrated therapeutic potential of Gal3 pseudotyped LV for targeted tumor cell killing through apoptosis mediated by the LV particle carrying mutSOD1 and Bcl2. He has also a developed a new platform with hygromycin resistance thereby increasing the options for multiple selection and gene delivery to same target cells. In summary, this thesis provides new insights and reported results are very useful in the context of translational research.

Publications

1. Dhamne H, Chande AG, Mukhopadhyaya R. Lentiviral vector platform for improved erythropoietin expression concomitant with shRNA mediated host cell elastase down regulation. Plasmid. 2014; 71:1-7
2. Chande AG, Raina S, Dhamne H, Kamat RH, Mukhopadhyaya R. Multiple platforms of HIV-2 derived Lentiviral vector for expanded utility. Plasmid. 2013; 69:90-5. Hemant Dhamne

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Enrolment No.	:	CHEM02200804011
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Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	Studies on the Molten Salt Electro-Deoxidation of Niobium, Titanium, Silicon and Uranium Oxides

Abstract

The process of direct oxide electrochemical reduction (DOER) of solid metal oxides to metals in molten salts is a recent development in the area of pyro-electrometallurgy. In this process, the metal oxide is converted to the metal via electrolysis by the application of a potential between the metal oxide (cathode) and graphite (anode) in a suitable molten salt electrolyte medium. A number of metal oxides such as TiO_2, Cr_2O_3 etc. have been converted to the respective metals by this process. Since the process is a new one, many fundamental issues still remain unexplored. The thesis focuses on the study of the fundamental aspects of the DOER of Nb_2O_5, TiO_2, SiO_2 and UO_2 in various molten salts. The thesis is segmented into 7 chapters, whose contents are described below.

Chapter 1 introduces the DOER process and discusses briefly the results of studies reported in literature, the discrepancies observed there in and the potential areas to be explored. Chapter 2 gives an account of the experimental aspects associated with the DOER process such as the preparation of salt, cathode, anode and reference electrode, assembling of the cell etc. in addition to the analytical techniques employed to characterise the products after electrolysis such as XRD, SEM-EDX and oxygen analysis. Chapter 3 brings out the fundamental issues of the DOER process taking Nb_2O_5 as the candidate oxide. The electrolysis experiments were carried out for different durations of time and the chemistry of the melt was studied by analyzing the same. From the results of XRD, SEM-EDX, electrochemical data and the melt analysis, the pathways of reduction of Nb_2O_5 were determined. The effects of the factors influencing the electrochemical reduction such as time of electrolysis, temperature, applied voltage, open porosity of pellets, mode of electrolysis, configuration of the cathode, composition of melt etc. were also determined. Chapter 4 deals with the electrochemical reduction studies carried out on TiO_2 and SiO_2 pellets particularly to investigate the effect of the conducting nature of the oxide on DOER. The results showed that TiO_2 pellet acted as a conductor by itself whereas SiO_2 pellet strictly followed three phase interline (conductor-oxide-melt) mechanism during electrochemical reduction. Electrochemical reduction studies were also carried out on TiO_2 powder sintered at 1423 K and 1673 K in molten $CaCl_2$. The reduction was found to be better with the powder sintered at 1423 K. In Chapter 5, the electrochemical reduction studies carried out on UO_2 were discussed. Analysis of the partially reduced samples from experiments, carried out in $CaCl_2$-48mol.% NaCl melt at 923 K, showed that the electrochemical reduction of UO_2 to U metal occurred directly without the formation of ternary intermediate compounds and sub-oxides of uranium. The rate of electrochemical reduction increased with increase in time of electrolysis, temperature, applied voltage and open porosity of pellets whereas it decreased with increase in temperature from 923 K to 1173 K. This was attributed to the sintering of the uranium metal to form a nonporous layer on the surface of the pellets. Studies carried out in LiCl-KCl-$CaCl_2$ melt at 673 K established that the reduction of UO_2 is feasible in the melt. Chapter 6 is dedicated to the

development of a new method for the determination of the extent of reduction in the partially reduced UO_2 samples obtained from DOER studies. The method is based on the use of a fuel cell type, polymer electrolyte based, hydrogen sensor for the online measurement of the hydrogen released during the dissolution of uranium metal from partially reduced U-UO_2 mixtures in acid. From the amount of the liberated hydrogen, the amount of uranium metal in the sample and hence the extent of reduction of UO_2 was determined. Chapter 7 summarises the results of all the chapters and projects some unexplored areas where there is a scope for further work.

Publications

International Journal Publications

1. D. Sri Maha Vishnu, N. Sanil, N. Murugesan, L. Shakila, C. Ramesh, K.S. Mohandas, K. Nagarajan, 'Determination of the extent of reduction of dense UO_2 cathodes from direct electrochemical reduction studies in molten chloride medium', Journal of nuclear materials, 427 (2012) 200-208.
2. D. Sri Maha Vishnu, N. Sanil, L. Shakila, G. Panneerselvam, R. Sudha, K.S. Mohandas, K. Nagarajan, 'A study of the reaction pathways during electrochemical reduction of dense Nb_2O_5 pellets in molten $CaCl_2$ medium', Electrochimica Acta, 100 (2013) 51-62.
3. D. Sri Maha Vishnu, N. Sanil, G. Panneerselvam, R. Sudha, K.S. Mohandas, K. Nagarajan, 'Mechanism of direct electrochemical reduction of solid UO_2 to uranium metal in $CaCl_2$-48mol%NaCl melt', Journal of the Electrochemical Society, 160 (9) (2013) D394-D402.
4. D. Sri Maha Vishnu, N. Sanil, G. Panneerselvam, S.K. Mahato, K.V. Soja, K.S. Mohandas, K. Nagarajan, 'Factors influencing the direct electrochemical reduction of UO_2 pellets to uranium metal in $CaCl_2$-48mol%NaCl melt', Journal of the Electrochemical Society, 160 (11) (2013) D583-D592.
5. N. Murugesan, D. Sri Maha Vishnu, N. Sanil, C. Ramesh, K. Nagarajan, V. Ganesan, 'A novel technique for estimation of metallic uranium using proton exchange membrane based hydrogen sensor', Transactions of Indian Institute of Metals (In press, DOI: 10.1007/s12666-014-0391-x).

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2. D. Sri Maha Vishnu, N. Sanil, L. Shakila, K.S. Mohandas, K. Nagarajan, Galvanostatic Electrodeoxidation of niobium pentoxide in molten calcium chloride medium, Proceedings of 3rd International Symposium on Materials Chemistry (ISMC), Bhabha Atomic Research Centre, Trombay, Mumbai, December 7-11, 2010, p. 135 (Won Best Paper Award).
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Name	:	**Sumeer Raina**
Enrolment No.	:	LIFE09200704004
Date of Award of degree	:	25.09.14
Constituent Institute	:	Tata Memorial Centre, Mumbai
Title	:	Lentiviral Vector Mediated Gene Transfer as an Antiviral and Antitumoral Intervention Strategy

Abstract

Lentiviral Vectors have emerged as promising tools for gene delivery for both in vitro and in vivo studies. Our laboratory earlier reported development of an Indian HIV-2 isolate derived LV with a novel versatile MCS; the isolate was also propagated in this laboratory. In the present thesis, we report use of this LV for targeted gene delivery and other modifications in the LV backbone to expand its potential utility.

We have achieved targeted gene delivery into specific cell types by engineering LV with chimeric molecules, receptors/co-receptors and envelope proteins from other virus. A novel envelope was developed by fusion of Galectin-3 and VSV-G transmembrane domain and LV pseudotyped using this envelope was shown to efficiently transduce B16F10 cells. Using a B16F10 mouse melanoma mouse model, we acheived targeted reporter gene delivery into the desired cells. Using HIV entry receptors like CD4/CXCR4 and/or CCR5 as envelopes for pseudotyping LV, HIV envelope expressing cells (HIV 1 infected SupT1 cell line) was specifically targeted and transduced with no transduction in the uninfected cells. Envelope proteins of HHV6 (light and heavy chain envelope glycoproteins) were successfully utilised to pseudotype LV. These pseudotyped LV showed selective tropism for SUPTI (T cell line) with moderate transduction efficiency and good stability even after concentration by ultra-centrifugation.

In the second part, we report the first LV derived single step assay for evaluation of drug candidates that can potentially inhibit HIV replication by interfering with Rev-RRE mediated HIV mRNA transport. This antiviral screening assay ensures that the only manipulation required in the assay is addition of the putative interfering drug which ensures complete bypassing of the time

consuming transfections/ co-transfections or cell viability based assay. Two compounds, PRF and K-37 were used to prove the efficacy of the assay. Availability of a cell line with LV integrated indicator constructs offers a selection free cell line and both the drugs showed similar end point profiles confirming the specificity of this assay.

Another study was aimed at generation of a regulatable platform for controlled gene expression of our HIV-2 vector. To achieve this, a drug inducible single LV construct was developed and stable cell lines were generated using these inducible constructs. The efficiency of the constructs was confirmed by regulated expression of the reporter genes in the presence of the doxycycline.

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2. Chande AG, Raina S, Dhamne H, Kamat RH, Mukhopadhyaya R. Multiple platforms of a HIV-2 derived Lentiviral vector for expanded utility. Plasmid. 2013, 69:90

Name : **Amalendu Sharma**
Enrolment No. : PHYS03200804003
Date of Award of degree : 25.09.14
Constituent Institute : Raja Rammana Centre for Advanced Technology, Indore
Title : Optics Design and Optimization of Electron Bunch Compressor Transfer Line (with a Case Study of CTF3 Bunch Compressor)

Abstract

The aim of the thesis is the beam optics design of a transfer line (Transfer Line-2) for CTF3 at CERN with the ability to compress the electron bunch length under the given constraints. A study of different optics usually employed for bunch length compression is also carried out.
The optics of bunch compressors are studied for two different cases i.e. in one case, the exit beam from bunch compressor is along the same axis as of the incoming beam in the bunch compressor and second case includes where the exit beam is shifted parallel from the incoming beam. In first case, a very general optics often employed is the chicane optics. But in this optics, R_{56}, which is the major optical parameter to compress the bunch length, has a fixed value. In thesis, by including quadrupole magnets in chicane optics tuning range of R_{56} is analyzed along with its chromatic behavior. Thesis also includes similar studies of two different arcs, in which beam at the exit is shifted parallel to the axis of incoming beam.

The thesis focuses on a design of beam optics, carried out for Transfer Line-2 (TL-2) of CTF3 for a very wide tuning range of R_{56} (-0.30 m to +0.30 m) to compress the bunch length. The design satisfies all the requirements of CERN, which also include utilization of available magnets and installation of the line in a given geometry of the pre existing building. The bunch length at the entrance of the line is 8.3 ps, which is to be compressed to ~1.5 ps.

At such short bunch length, second order effects of the magnetic optics also become important. Bunch length can be deteriorated by the second order aberration in optics and major second order aberration for bunch length deterioration is T_{566}. In order to correct T_{566}, a new sextupole scheme has been evolved and has been applied successfully in entire range of R_{56} tuning in this transfer line, keeping dilution in transverse emittance below 10%.

When electron travels in a curved path inside the dipole magnet, it emits synchrotron radiation. At shorter bunch length, the emitted radiation can become coherent. Coherent Synchrotron Radiation (CSR) can increase the bunch length and also can dilute the transverse emittance. Detailed simulation studies are carried out to quantify the effect of CSR on bunch length and

transverse emittance in TL-2, which is found to be insignificant in the domain of operation of this line.

In addition, the exact analytical expressions of transfer functions of a hard edge dipole magnet using a basic geometrical approach has been derived. This new formulation shows that higher order effects are more pronounced in longitudinal plane and therefore have more importance for the optics of bunch compressors. Application of these expressions to chicane type bunch compressors shows deviation in results for bunch length obtained using computer codes which simulate up to third order. This expression can be used in quick estimation of bunch length and emittance more accurately.

Publications

Journal

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Others

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Name	:	**Gangamallaiah Velpula**
Enrolment No.	:	CHEM01200904016
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Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	Solute Rotation and Photoisomerization in Complex \ Fluids

Abstract

To comprehend how the complex and diverse environments of ionic liquids and reverse micelles influence processes such as solute rotation and photoisomerization the present work has been undertaken. This thesis examines rotational diffusion of a pair of structurally similar nonpolar and ionic solutes in 1-alkyl-3-methylimidazolium-based ionic liquids with strongly and weakly associating anions. The results have been analyzed with the aid of Stokes-Einstein-Debye hydrodynamic and quasihydrodynamic theories and the observed deviations have been explained by considering the organized structure of these ionic liquids. In the case of imidazolium-based ionic liquids with strongly associating anions, the influence of organized structure on solute rotation has been observed. However, in case of weakly associating anions, the affect of organized structure on solute rotation becomes significant only when the number of

carbon atoms in the alkyl chain attached to imidazolium cation exceeds eight. Besides these rotational diffusion studies, photoisomerization studies have been investigated in ionic liquids to find out whether the process of photoisomerization of carbocyanine derivative is different compared to that observed in conventional solvents and also test the applicability of Kramers model. As in case of alcohols, the isomerization data could not be explained by the hydrodynamic Kramers model. Therefore, to improve agreement between experiment and theory, frequency dependence of the medium needs to be considered. The factor of two higher activation energy obtained for solute isomerization in ionic liquids compared to alcohols is probably due to the organized structure of the medium, which hinders the excited-state twisting motion. Apart from ionic liquids, photoisomerization of carbocyanine derivatives has been carried out in AOT reverse micelles to identify the parameter that characterizes interfacial friction. An inverse correlation has been obtained between nonradiative rate constants and critical packing parameter, indicating that the interfacial friction experienced by the solute molecule is essentially described by this parameter.

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6. Effect of alkyl chain length on the rotational diffusion of nonpolar and ionic solute

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Title	:	Mode of Action of Two Aureolic Acid Antibiotics and Chelerythrine - A Chemical Biology Approach

Abstract

Present thesis aims to understand the chemical biology of action of two aureolic acid antibiotics, mithramycin (MTR) and chromomycin A3 (CHR) and one plant alkaloid, chelerythrine (CHL).Physico-chemical properties of antibiotics like the size and shape of antibiotics, degree of ionization, state of aggregation play important roles in their mode of action. Studies of the association of these small molecules with the potential cellular targets also throw light on their mode of action.

The 1st chapter is a compact review of literature related to the above small molecules. Among them MTR and CHR have similar aglyconemoietybut differ in oligosaccharide side chains.The difference in ionization properties of the antibiotics, MTR and CHR was studiedby means of optical spectroscopic methods and calorimetric techniquesin 2ndchapter. Ionization constants

(pK_a) of MTR and CHR are 5.5 and 7.0, respectively. Different sugars and specific modifications of the sugars are responsible for the different ionization property of MTR and CHR.
In 3rdchapterself-associationof CHR inneutral and anionic forms has beenexamined by means of spectroscopic and calorimetric techniques. The mode of aggregation was also characterized by ^{1}H NMR studies.Oligomerization of neutral and anionic forms of CHR starts at low concentrations and sugar moieties play key roles in this process.

The 4thchapter focuses onthe association of a biologically important divalent transition metal ion, Mn^{2+}, with MTR. The association leads to formation of complex,[$(MTR)_2$ Mn^{2+}]. The complex binds to chromatin and chromosomal DNA.The association process has been examined. The effect of the MTR upon properties of the metalloenzyme, MnSOD, has been studied.

In 5thchapter the binding of chelerythrine (CHL)with chromosomal DNA and four synthetic polynucleotides, poly(dG-dC), poly(dG).poly(dC), poly(dA-dT) and poly(dA).poly(dT), are studied. The results show that association of CHL with polynucleotide is sequence dependent. Studies on the association of CHL with chromatin and its components show that the presence of associated histone proteins in chromatin and chromatosome has a negative effect upon DNA-binding potential of CHL.The results help us to understand an additional mode of action of CHL.

Publications

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2. "Association of antitumor antibiotic Mithramycin with Mn^{2+} and the potential cellular targets of Mithramycin after association with Mn^{2+}",ShreyasiDutta, ShibojyotiLahiri, Amrita Banerjee, ShriyaSaha and DipakDasgupta, Journal of Biomolecular Structure and Dynamics,2014, DOI: 0.1080/07391102.2014.887031

Communicated

3. 1.

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1. "Association of antitumor antibiotic Mithramycin and Chromomycin A3 with Mn^{2+}",ShreyasiDutta and DipakDasgupta, Recent advances in chemical and physical biology,2012, SahaInstitute of Nuclear Physics, Kolkata.
2. "Association of Mithramycin with essential trace element Cu^{2+} and its interaction with metalloenzymes Cu/Zn Superoxide dismutase (SOD1) and metallo β-Lactamase (MBL)",ShibojyotiLahiri,ShreyasiDuttaand DipakDasgupta,Recent advances in chemical and physical biology, 2012, SahaInstitute of Nuclear Physics, Kolkata.
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4. "Association of antitumor antibiotics Mithramycin with Mn^{2+} and biological significance of the association",ShreyasiDutta and DipakDasgupta, Photosciences: Contemporary Challenges and Future Perspectives, 2013, Jadavpur University, Kolkata

Name	:	**Md. Zahid Kamran**
Enrolment No.	:	LIFE09200804014
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Constituent Institute	:	Tata Memorial Centre, Mumbai
Title	:	Effects of Methylxanthine on STAT3 Mediated Regulation of Cytokines Involved in Tumor Development and Tumor Induced Sugiogenesis in Melanoma Cells

Abstract

Metastasis, rather than the primary tumor is the major cause of mortality in majority of cancer patients. To cut down this mortality, improved ways or novel therapies are urgently needed. Pentoxifylline (PTX), a non-specific phosphodiesterase inhibitor, is a FDA approved drug for treatment of peripheral vascular disease. The present work unravels the anti-metastatic and anti-angiogenic effects of PTX with underlying molecular mechanism in human A375 melanoma cells. Despite minimal toxicity to normal cells, PTX at sub-toxic doses inhibited cellular growth and proliferation of cancer cells by inhibiting cell cycle progression from G1/S phase and also by induction of apoptosis. Cells treated with PTX showed an inhibition in adhesion to ECM substrate matrigel and type IV collagen. Activity of MMP2 and MMP9 was decreased on PTX treatment. Cell treated with PTX showed abnormalities in cytoskeletal structures and impaired cellular migration. STAT3 is constitutively activated in majority of human cancers and regarded as a druggable target. PTX inhibited constitutive as well as IL6-inducible STAT3 activation in a dose dependent manner. This inhibition was partly mediated through the inhibition of upstream kinases pJAK1 and pJAK2. PTX also inhibited STAT3 nuclear translocation and binding of STAT3 to DNA. Expression of various STAT3 regulated gene products, such as cylinDl, cMyc, BclXl, HIFa, VEGF, MMP2 and MMP9 were downregulated following PTX treatment. Further investigation of the underlying mechanism revealed that PTX inhibited pp38 MAPK, SAPK/JNK and pAkt expression. PTX treatment significantly inhibited solid tumor growth induced by sub-cutaneous route in vivo and also inhibited tumor induced angiogenesis in intra-dermal xenograft model.

Publications

1. Mohammad Zahid Kamran, Rajiv P. Gude. Pentoxifylline inhibits melanoma tumor growth and angiogenesis by targeting STAT3 signaling pathway. Biomedicine & Pharmacotherapy, 67 (2013) 399-405.
2. Mohammad Zahid Kamran, Rajiv P. Gude. Preclinical evaluation of the antimetastatic efficacy of Pentoxifylline on A375 human melanoma cell line. Biomedicine & Pharmacotherapy, 66 (2012), 617-626.\
3. Mohammad Zahid Kamran, Prachi Patil, Rajiv P. Gude. Role of STAT3 in Cancer Metastasis and Translational Advances. BioMed Research International, Volume 2013, Article ID 421821, 15 pages, http://dx.doi.org/10.1155/2013/421821.
4. Mohammad Zahid Kamran, Prachi Patil, Kavita Shirsath, Rajiv P. Gude. Tyrosine Kinase inhibitor AG490 inhibits the proliferation and migration and disrupts actin organization of cancer cells. Journal of Environmental Pathology, Toxicology and Oncology, 32 (2013), 361-371.

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1. Mohammad Zahid Kamran, Rajiv P. Gude. Pentoxifylline as an inhibitor of oncogenic signaling pathways: molecular mechanism and clinical implication. Signaling and acquired resistance to targeted cancer therapeutics. 5-7 January, 2014, Robinson College, University of Cambridge, United Kingdom, (Poster presentation).
2. Mohammad Zahid Kamran, Rajiv P. Gude. Hemorrheological agent Pentoxifylline modulates oncogenic signaling pathways: an old drug with new perspectives. Current Advances in Immunobiology and Cancer. 28-30 November, 2013, Mumbai, India, (Poster presentation).

3. Mohammad Zahid Kamran, Rajiv P. Gude. Novel mechanistic insights for phosphodiesterase inhibitor Pentoxifylline: as a STAT3 inhibitor. 4th International Conference on Stem Cells and Cancer (ICSCC-2013): Proliferation, Differentiation, and Apoptosis. 19 - 22 October, 2013, Mumbai, India, (oral presentation).
4. Mohammad Zahid Kamran, Rajiv P. Gude. Pentoxifylline inhibits melanoma tumor growth and angiogenesis by targeting STAT3 signaling pathway: Novel mode of action(s) for an old drug. 81st Annual meeting of the Society of Biological Chemist (I). 8-11 November, 2012, Kolkata, India, (poster presentation).
5. Mohammad Zahid Kamran, Rajiv P. Gude. Pentoxifylline inhibit melanoma angiogenesis via STAT3 signaling pathway. AACR International Conference: New Horizons in Cancer Research: Biology to Prevention to Therapy. 13-16 December, 2011, New Delhi, India, (poster presentation).

Name	:	**Ramakanta Mahakud**
Enrolment No.	:	PHYS03200904003
Date of Award of degree	:	10.10.14
Constituent Institute	:	Raja Rammana Centre for Advanced Technology, Indore
Title	:	Studies on Fabrication of Fiber Bragg Gratings Using High Repetition Rate Ultraviolet Radiation from Frequency Converted Copper Vapour Laser

Abstract

Fiber Bragg gratings (FBGs) are written by inducing refracting index modulation in the fiber core. The present thesis comprises of experimental and analytical works on the FBG fabrication by 255 nm UV beams. The high repetition rate (5.6 kHz) and low pulse energy (~ 50pJ) UV beams of nano-second duration (20-30 ns) were generated from second harmonic (SH) of copper vapour laser (CVL, 510 nm). An efficient FBG inscription set up has been developed and utilized for fabrication of type I, type IIA and tilted FBGs in Ge-doped and Ge- B co-doped single mode fibers. The FBG fabrication was theoretically analyzed. The FBGs were stabilized by thermal annealing for application in high temperature sensing.

The UV beams of different spatial characteristics were generated from SH conversion of CVL in unstable and filtering resonators. Various CVL/UV beam parameters were studied. Experiment and analysis were carried out to study the effect of UV beam pointing stability and spatial coherence on contrast and stability of UV fringes and subsequently on FBG writing. The FBG growth characteristics were studied. The growth and saturation of refractive index modulation changed with change in fibre composition and UV beam coherence. A physical model of photo-induced refractive index modulation incorporating fringe contrast was used to analyze and explain the observed results. This model was further extended by incorporating UV beam energy distribution and its focusing to explain the dynamic evolution of reflection spectrum during FBG inscription. The model facilitated the active control of the FBG writing and post fabrication processing. The FBGs of different length (2 mm to 10 mm), bandwidth (0.2 nm to 1 nm) and reflectivity (up to maximum of 99.98 %, 38 dB) have been written, in times as short as few minutes. The FBG writing was also carried out by a biprism interferometer. This technique is cost effective and convenient choice for Bragg wavelength tuning. Numerical analysis was carried out for maximizing the FBG reflectivity and wavelength tuning. It is analytically shown that the fiber position of maximum reflectivity in biprism fringe depth is dictated by the UV beam divergence, beam radius and biprism refraction angle. The observed FBG reflectivity of 99.7 % (~ 12 dB) is one of the highest reported for biprism based writing. Thermal response of FBGs were studied in the temperature range of 25 ^{0}C to 900 ^{0}C. The observed temperature sensitivity of a typical FBG was of the order of 11 pm/^{0}C. However, the temperature sensitivity increased with increase in temperature. This was different for FBGs written in different fiber types. A theoretical analysis was carried out on the factors affecting the shift of Bragg wavelength with change in temperature. It demonstrated that the non-uniform behavior of temperature sensitivity in a bare

FBG is the combined effect of thermal expansion coefficient of fiber and temperature derivatives of effective refractive index. The temperature sensitivity of embedded FBGs increased with the increase in fractional strain transfer from the substrate. The FBGs in Ge-B co doped fiber sustained temperature up to about 600 ^{0}C- 650 ^{0}C. In contrast, the Ge-doped fiber sustained temperature up to ~ 900 ^{0}C. Based on these studies, FBG based single point high temperature sensors have been developed. It is analyzed the lower thermal release rate and higher energy depth of trapped population in Ge-doped FBGs leads to higher temperature sustainability.

Overall, this thesis work consists of eight chapters. The work arising from the present thesis led to about 10 publications in referred journals of high repute, supplementing a very limited literature available in FBG fabrication using high repetition rate 255 nm UV sources.

Publications

Journal

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3. "Analysis on the effect of UV beam intensity profile on the refractive index modulation in phase mask based fiber Bragg grating writing" R. Mahakud, O. Prakash, J. Kumar, S. V. Nakhe and S. K. Dixit, Optics Communications, 2012, 285, 5351-5358.
4. "Analysis on the saturation of refractive index modulation in fiber Bragg gratings (FBGs) written by partially coherent UV beams", R. Mahakud, O. Prakash, S.V. Nakhe and S. K. Dixit, Applied Optics, 2012, 51, 1828-1835.
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6. "Enhanced temperature (~ 800 ^{0}C) stability of type IIa fiber Bragg grating written in Ge doped photosensitive fiber", O. Prakash, J. Kumar, R. Mahakud, S. K. Agrawal, S. K. Dixit and S. V. Nakhe, IEEE photonics technology letters, 2014, 26, 93-95.
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10. "Effect of pulse to pulse variation of divergence, pointing and amplitude of copper vapour laser radiations on their second harmonic and sum frequency conversion" O. Prakash, R. Mahakud, S. V. Nakhe and S. K. Dixit, Optics & Laser Technology, 2013, 50, 43-50.
11. "Comparative study on second harmonic conversion and saturation characteristics of three copper vapor laser beams of same average power and different spatial coherence", O.Prakash, R. Mahakud and S.K. Dixit, Optical Engineering, 2011, 50, 114201-6.
12. "Role of optical resonator on the pointing stability of copper vapour laser" S. K Dixit, R. Mahakud, O. Prakash, R. Biswal and J. K. Mittal, Optics Communications, 2008, 281, 2590-2597.

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Enrolment No.	:	LIFE03200704001
Date of Award of degree	:	10.10.14
Constituent Institute	:	Raja Rammana Centre for Advanced Technology, Indore
Title	:	Studies on the Evaluation of Photodynamic Efficacy of Chlorophyll Derivatives in Cancer Cells and Animal Tumor Model

Abstract

The thesis deals with studies on the evaluation of the efficacy of Chlorin p_6-histamine conjugate (Cp_6- his) for photodynamic treatment (PDT) of cancer. These include (i) In-vitro studies on uptake and phototoxicity of Cp_6 and Cp_6-his in oral cancer cell lines. Results showed that the cellular uptake of Cp_6-his was ~10 times higher than free Cp_6 and the photo-toxicity is enhanced by a factor of ~4. The expression of histamine H2 receptors in oral cancer cells and involvement of these receptors in uptake of Cp_6-his is also confirmed, (ii) Investigations on intracellular localization of Cp_6-his. The results revealed that the primary target sites of Cp_6-his are endoplasmic reticulum (ER) and lysosomes which suggested that its uptake is mediated by endocytosis. (iii) In-vivo studies on use of Cp_6-his mediated PDT of chemically induced tumor in hamster cheek pouch. These studies showed that as compared to Cp_6, the tumor selectivity of Cp_5-his was ~ 4 times higher and the tumors of size <1000 $mm^{6\,7}$ regressed completely after PDT whereas, for Cp_6 complete tumor regression was seen for tumors of size <150 mm^3. Results also showed that Cp_6-his clear rapidly from the skin due to which skin photosensitivity is expected to be less. These results suggested that conjugating Cp_6 to histamine is useful for improving the PDT efficacy of Cp_6. (iv) Studies on mode of transport and metabolic clearance of C/?$_6$-his. Results showed that as compared to Cp_6, the biding affinity of Cp_6-his with serum albumin is lower which would improve its bioavailability and thus may also contribute to higher uptake in tumor. Further, the inhibition of Cytochrome P450 enzymes by C/?$_6$-his was observed to be significantly lower than that reported for protoporphyrin. This would imply faster clearance and lower liver toxicity.

Publications

Journals:

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2. Photodynamic treatment of oral squamous cell carcinoma in hamster cheek pouch model using chlorin p6-histamine conjugate. A. Parihar, A. Dube and P. K. Gupta. Photodiagnosis and Photodynamic Therapy, 2013, 10:79-86.

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2. Conjugation of Chlorin p6 to histamine enhances efficacy of photodynamic treatment in human breast cancer cells. A. Parihar, A. Dube and P. K. Gupta. “8th International Symposium on Photodynamic Therapy and Photodiagnosis in Clinical Practice” (05-09 Oct., 2010) University of Padova, Brixen, Italy.
3. Evaluation of photodynamic efficacy of Chlorin p6-histamine conjugate in oral cancer cell lines. A. Parihar, A. Dube, P.K. Gupta. “National Symposium on Frontiers in Photobiology” 24-26 Aug., 2009) BARC, India.

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Title	:	Risk Factors of Breast Cancer in Rural & Urban India

Abstract

It has been observed for long time that the rates of BC differ in rural and urban areas. However, there are very few studies in literature to address the reasons for the differences in BC rates of rural and urban area. Obesity has been observed to be risk factor for postmenopausal BC. However the contribution of different measures of obesity and their role in pre- and postmenopausal women is still not clear. In Indian context, there are no large studies to address the issue of reproductive factors, obesity, age at last pregnancy, OC use in development of BC. Though there has been large GWAS on BC in most developed countries showing low to modest associations between common polymorphisms and BC risk. In India, however, there have been no GWAS and few properly designed retrospective studies with smaller sample size on genetic susceptibility to study this risk.

The present thesis proposal is designed to understand more clearly the reasons for rural-urban differences, and role of genetic susceptibility in development of BC.

Methodology : A hospital based case-control (female visitors) study was conducted at Tata Memorial Hospital (TMH), Mumbai during the period of January 2009 to September 2013 with information collected on residential status, reproductive history and anthropometric measurements. ER, PR and Human Epidermal Growth Factor Receptor 2 (HER2) status were obtained from hospital pathology records. 10ml blood sample was collected from each study participant and centrifuged into plasma and buffy coat. DNA extracted from buffy coat were then genotyped for 384 SNPs in Illumina Hi-Scan.

Results & Discussion : A total of 1637 cases and 1515 controls were enrolled in the study. A statistically significant protection in risk of BC was observed in women who lived for first twenty years of life in rural area as compared to women who lived less than 20 years in rural area, as exposures in early life may be more important in the development of BC compared to current exposures. A statistically significant difference (P = 0.018) in the prevalence of TNBC tumours was observed in women who have lived first twenty years of life in rural area (44.21%) as compared to women who have lived less than 20 years in rural area (34.39%). The risk of BC significantly increased with every 2 year delay in pregnancy after age 25 in women from both urban and rural areas. On stratifying into menopausal status, statistically significant association was observed only in premenopausal women, while the postmenopausal women showed increase but statistically non significant risk. This is possibly because of homogeneity of population in relation to age at first pregnancy in older cohort where the median age at first child birth is lower as compared to the women from newer cohort. The current OC users using OC for more than 2 years showed increased risk for urban women compared to women without use of OC (OR = 2.46; 95% Cl: 0.99-6.12). The association may be interpreted as causal in urban India. As the association was significant only for current users, it can be interpreted that OC may act as late-stage promoters.

A protective association observed in premenopausal women (OR = 0.93; 95% Cl: 0.91-0.95) with per unit increase in BMI (world) continued in women who had attained menopause less than 10 years ago (OR = 0.95; 95% Cl: 0.92-0.98). No increase in risk in postmenopausal BC could be observed possibly because of carry-over protective effect. A strong significant increase (OR =1.85; P = 0.03) with dose-response was observed for women with high BMI who attained menopause > 10 years ago from the date of

enrolment. With every 0.1 increase in WHR the risk of BC increased (OR = 1.76; 95% Cl: 1.55-2.01), (OR = 1.55; 95% Cl: 1.29-1.86) (OR = 1.69; 95% Cl: 1.47-1.96) and (OR = 1.71; 95% Cl: 1.41-2.00) in urban, rural, premenopausal and postmenopausal women respectively. In the present study the prevalence of WHR was higher in women residing in urban as well as rural areas. Even with women for normal BMI, 34.4% had higher WHR in the present study. This is consistent with thin-fat hypothesis of Asian -Indians [287], In the present study, for every 5 cm increase in height the OR of 1.10 (95% Cl: 1.02-1.19) was observed in the urban area and in premenopausal women (OR = 1.24; 95% Cl: 1.12-1.37), but not in rural area (OR = 1.05; 95% Cl: 0.93-1.19) possibly because of the low prevalence of taller women in rural areas.

The present study could replicate 7 SNPs from BC GW AS. Five SNPs were successfully replicated out of 42 Candidate SNPs of BC used for analysis. SNPs selected from FGFR2 gene were positively associated with BC. 25 SNPs which were identified as a risk factor for BC in the GWAS conducted in other populations did not replicate in the Indian population, even though their prevalence was high (> 20%) indicating that they may not be a risk factor in Indian population. The 3 SNPs which were highly prevalent in GWAS population could not be replicated even if they were associated the attributable risk of the SNPs remains low due to their low prevalence in the present study population. The genetic susceptibility of SNPs associated with BMI and obesity in various GWAS were associated with BC risk suggesting that BC is mainly driven by genes related to obesity. Fourteen SNPs selected using Bioinformatics tool from candidate genes associated with obesity were first time identified to be strongly associated with the BC risk and hence need further validation.

Conclusion : current study demonstrates that protection observed for BC by living in a rural area is possibly because of less prevalence of risk factors viz. late age at first full-term pregnancy,

OC use and tallness. The central obesity common to both rural and urban is a strong risk factor for BC. The study was successful in identifying new SNPs in obesity genes identified using Bioinformatics tool, however their association would have to be replicated in other studies particularly because they were not significant after adjusting for multiple comparisons. This also indicates that the lifestyle factors are more important than the genetic markers from public health point of view.

Publications

Journal

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Title	:	Study of Long-Term Behaviour of Actinides in the Tropical Marine Ecosystem of Trombay

Abstract

The work carried out under this dissertation deals with interaction of three important members of the actinides i.e. Uranium (U), Thorium (Th) and Plutonium (Pu) in the marine ecosystem of Mumbai Harbour Bay. The activity concentrations of U, Th and $^{239+240}$Pu in seawater were ranged from 1 - 4.4 µg L^{-1} (mean: 2.6 ± 0.83 µg L^{-1}), 70 – 250 ng L^{-1} (mean: 143 ± 51 ng L^{-1}) and 47 – 138 µBq L^{-1} (mean: 86 ± 30 µBq L^{-1}) respectively. These levels are on lower side compared to others equivalent scenario internationally like La hague, France and Sellafield, UK reprocessing. Whereas in case of bottom (grab) sediments, concentrations of ^{238}U, ^{232}Th and $^{239+240}$Pu in bottom sediments of all locations ranged from 8.5 to 14 Bqkg^{-1}, dry (mean:11.5 ± 1.7 Bq kg^{-1}, dry), 21.5 to 61.2 Bq kg^{-1}, dry (mean: 40 ± 11.4 Bq kg^{-1}, dry) and 0.16 to 1.5 Bq kg^{-1}, dry (mean: 0.7 ± 0.4 Bq kg^{-1}, dry). The spatial variability of ^{238}U, ^{232}Th and $^{239+240}$Pu in terms of coefficient of variation (CV) throughout the studied area has been found to be 15.4%, 28.5% and 63 %. Experimental results clearly indicates that distribution of ^{238}U, ^{232}Th and $^{239+240}$Pu in the marine ecosystem is highly influenced by the concentration profiles of major and minor elements in different matrices of marine ecosystem. k_d values were evaluated under different geochemical conditions to understand the role of sediments in scavenging and removing radionuclides from the aquatic systems. The sorption parameters of U and Th obtained from the experimental results for sediment-seawater and soil-groundwater systems were fitted to Freundlich, Linear and Langmuir models. Thermodynamic parameters were evaluated to understand the sorption of uranium onto sediment in seawater and compared with other geochemical environments such as soil – groundwater/deionised water. The negative value of ΔGº and positive value of ΔHº reflects that sorption of uranium onto both sediment/soil systems are a spontaneous and endothermic process under experimental conditions. The speciation of U, Th and Pu at various physico-chemical parameters of marine environment was calculated by the speciation code MEDUSA. This code includes an extensive thermodynamic data base along with HYDRA (hydrochemical equilibrium constant database) speciation program and three main different algorithms for creating chemical equilibrium diagrams. The ligands such as hydroxide, chloride, nitrate, carbonate, fluoride, sulphate, phosphate and silicate are included. Since there are many constraints while working with Pu as the concentration were very small, therefore various conclusions were drawn on the basis of uranium.

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2. A novel approach to determine the recent sedimentation rate in the Mumbai Harbour Bay using ^{228}Ra/^{226}Ra geochronology, Ajay Kumar, Sabyasachi Rout, Manish K. Mishra, P.M. Ravi and R.M. Tripathi, (2014), National conference on Advances in Radiation Measurement Systems and Techniques, (IARPNC-2014), 19 – 21, March, 2014, BARC Trombay, Mumbai.
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4. Salinity effect and pH dependence of chemical speciation and kinetic rate of U (VI) sorption onto soil in groundwater system, Ajay Kumar, Sabyasachi Rout, Rupali Karpe and P.M. Ravi, (2013), National Symposium on Environment (NSE-18), Anantapur (AP), 11-12, March, 2013 (BS Publications, Hyderabad, ISBN:978-81-7800-287-3).
5. A Comparative study of distribution coefficients (K_d) for naturally occurring Uranium (U) and Thorium (Th) in two different aquatic environments, Ajay Kumar, Rupali Karpe, Sabyasachi Rout, Manish Kumar Mishra, Usha Narayanan and P.M. Ravi (2012), Radiation protection and environment. Indian Association of Radiation Protection (IARPNC-2012) , 15-17, March, 2012, Mangalore University, Mangalore.
6. Particle size characterization and distribution of Ra-226 and Ra-228 as a function of depth in Marine sediments, Ajay Kumar, Rupali Karpe, Sabyasachi Rout, Manish K. Mishra, V.M. Joshi and P.M. Ravi (2012), National conference of Indian Aerosol Science and Technology Association (IASTA-2012), 11 – 13, December 2012, Vashi, Navi Mumbai.
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Title	:	Studies on Radiation Induced Synthesis, Thermal Behavior and Applications of Polydiallyldime-thylammonium Chloride System

Abstract

Polydiallyldimethylammonium chloride (PDADMAC) is a cationic polyelectrolyte which has generated immense interest partly because of its unique polymerization chemistry which is relevant to fundamental studies and also due to its applications in many industries. Although a large number of polymers are processed by radiation for various applications, there is very little information available about the interaction of high energy radiation with DADMAC and PDADMAC. In this thesis, gamma radiation effect on DADMAC and its polymer; immobilization of PDADMAC for potential applications and PDADMAC assisted synthesis of gold nanoparticles were investigated. Detailed thermal characterization of DADMAC and radiation synthesized PDADMAC were also carried out

The reactions of the monomer and polymer with transient species produced by radiolysis of water, namely e_{aq}^- and *OH were studied in the nanosecond timescale by means of pulse radiolysis technique. Polymerization of DADMAC was initiated by gamma radiation and the various parameters affecting yield of the polymer were evaluated and subsequently, the polymer produced was characterized by various techniques such as UV-Visible, FT-IR, H-NMR and C- NMR. Based on the structural analysis of the polymer a mechanistic pathway for its formation was suggested. Thermal behavior of DADMAC and radiation synthesized PDADMAC were studied using TGA and DSC techniques and important kinetic parameters associated with the various phase transitions and decompositions of the polymer were evaluated. Based on these observations, a convenient thermogravimetric method was developed to determine the degree of conversion of DADMAC to PDADMAC during polymerization.

In order to realize the potential of quaternary ammonium group for practical applications, PDADMAC was immobilized on an inert support by two methods, namely, radiation induced grafting and a radiolytic encapsulation procedure. DADMAC was successfully grafted onto polyethylene substrate by employing a two step grafting procedure and many of the factors that exert a strong influence on the grafting yield were investigated. For immobilization of PDADMAC in the core of polyethersulfone microcapsule, a radiolytic process was developed and it was demonstrated that the functionalized microcapsule could absorb and exchange anions such as F, CP, Br, NO_3 " and SO_4 " at ppm level concentration.

In a part of the study, PDADMAC was employed as a capping agent for the synthesis of gold nanoparticles under gamma radiolytic conditions. Stable spherical gold nanoparticles and gold nanoparticles having triangular and hexagonal shapes could be synthesized in abundant yield by adjusting the experimental conditions. A photochemical method was also developed employing PDADMAC as the shape controlling capping agent. This method, in addition to producing the usual gold nanoplates, could afford the synthesis of concave nanoplates which are reported to be effective catalyst for various organic oxidation reactions.

Publications

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Title	:	Formality of Certain CW Complexes and Applications

Abstract

Let X be a simply connected space having rational homology of finite type. Suppose X is a formal space in the sense that its minimal model can be constructed from (H*(X; Q), 0). Let Y = X U_a e^n where a: S^{n-1} ^ X is a continuous map. In this thesis we obtain a criterion for formality of Y in terms of [a] £ n_{n-1}(X). In another direction, we consider maps between grass manifolds. Let $G_{n,k}$ denote the complex Grassmann manifold of all k-dimensional vector subspaces of C^n. Using the fact that any map f: $G_{n,k}$ ^ $G_{m>l}$ is formal, we shall show that the set [$G_{m>l}$, $G_{n,k}$] of homotopy classes of maps is finite if 1 < k < [n/2j ,1 < l < [m/2j ,k < l, m — l > n — k and m — l > $2k^2$ — k — 1 or 1 < k < 3. We obtain some applications of this result. we now give more precise statements of the main results of the thesis.

Theorem 1. Suppose that X is a simply connected space and is formal. Let = A(V) and suppose that V = ©fc>oV_k is a standard lower gradation of V. Let Y = X U_a e^n. Suppose that n([a]) = 0 so that j*(u) =: u = 0. (i) If [a] £ n_{n-1} (X) is a torsion element then u is indecomposable and Y is formal. (ii) Let [a] = 0 in n^Q_{-1}(X). Suppose that (v, [a]) = 0 for all v £ V_i G V^{n-1}, k =1, and that u is decomposable

in H*(Y; Q). Then Y is formal. (iii) If [a] £ n_{n-1}(X) is not a torsion element and u is not decomposable, then Y is not formal. In cases (i) and (ii), the inclusion i: X ^ Y is formal.

Theorem 2. Let 1 < k < [n/2_|, 1 < l < [m/2j and k < l, where m,n are positive integers such that m — l > n — k. Suppose that (i) m — l > $2k^2$ — k — 1 or 1 < k < 3. Then the set [$(G_{m>l})_0$, $(G_{n,k})_0$] of homotopy classes of continuous maps consists of only the class of constant maps and consequently the set [$G_{m>l}$, $G_{n,k}$] of homotopy classes of maps is finite

Publications

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3. Prateep Chakraborty and Parameswaran Sankaran, Errata: " Formality of certain CW complexes and applications to Schubert varieties and torus manifolds ", to apprear in J. Ramanujan Math. Soc. (arXiv:1301.5421).

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Title	:	Identified Particle Production in Pb-Pb and pp Collisions at LHC Energies

Abstract

The main goal of ultra relativistic heavy-ion collisons is to investigate the strongly interacting matter, called the Quark Gluon Plasma (QGP), expected to produce in such collisions. The Large Hadron Collider (LHC) at CERN provides a unique opportunity to study such strongly interacting matter at extreme energy densities.

The short lived resonances are very useful tool in high energy collisions to study the dynamics and properties of a strongly interacting medium. In particular, the K^{*0}(892) meson is important because its lifetime (4 fm/c) is comparable to the time scale of the hot and dense matter produced. Owing to short lifetime, the characteristic properties such as mass, width, yield and transverse momentum spectra of K*° is very sensitive to the dynamics and in-medium effects. Basically the decay products of K*°, the pions and kaons, may undergo in-medium effects. The decay products of high momentum resonances have a larger probability to escape the system and thereby detected, while that of low momentum resonances can be re-scattered by other hadrons present in the medium. Thus, we cannot reconstruct back the resonance and the signal is lost. On the other hand, the pions and kaons in the medium can re-generate K*° via pseudo-elastic interactions (Kn ! K*° ! Kn) during the phase between the chemical freeze-out (when inelastic collision ceases) and the kinetic freeze out (when elastic collision ceases). This re-generation process could compensate for the K*° yield, lost in re-scattering, if the system formed has a long expansion time. It was observed that the pion-pion interaction cross section is five times larger than the kaon-pion interaction cross section. The pion-pion interaction cross-section is responsible for the re-scattering, while the kaon-pion cross-section for the re-generation processes. Thus, the interplay of the two processes, re-scattering and re-generation, will decide the final resonance yield and a resonance to non-resonance particle ratio can be used to understand these processes. Since the K*° and K^- have different masses and spins, but they have identical quark content, the K*°/K^- ratio can be used as a tool to understand the re-scattering and re-generation processes in the hadronic phase. The production of K*° has been measured in STAR

experiment at RHIC, which shows the dominance of re-scattering effect over the re-generation mechanism. In this thesis, we will present the results of K^{*0} production via its hadronic decay channel (K*° ! $n^{-}K$ + and K^{*0} ! $n+K^{-}$) at mid rapidity (-0.5 < y < 0.5) in Pb+Pb collisions at s_{NN} = 2.76 TeV and in minimum bias p+p collisions at ɣ/s = 2.76 TeV. We will present the mass, width, yield and transverse momentum spectra of K*° meson. This will enable us to understand the in-medium effects and freeze-out conditions at unprecedented higher energies attained at the LHC. The mean transverse momentum (hp_T)) of K*° will be obtained and compared with other hadrons and lower energy measurements to investigate particle production mechanism at LHC energies. The particle ratio $K^{*°}/K^{-}$ will be obtained in different collision centralities in Pb+Pb collisions and minimum bias p+p collisions. It will also be compared with lower energy measurements at SPS and RHIC. Such results will shed light on the evolution of the hadronic medium formed at higher energies and one can estimate the lower limit of the lifetime of the hadronic interacting phase. Also, the $K^{*°}/K^{-}$ ratio will be compared to $0/K^{-}$ ratio, which is expected to be less affected by the hadronic interactions since the lifetime of 0 is about 10 times longer than that of K*°.

The nuclear modification factor R_{CP} (ratio of yields of K*° in central to those in peripheral collisions and appropriately normalized by the number of binary collisions) or R_{aa} (scaled to p+p collisions) are the variables to study the effect of the medium on $K^{*°}$ production in heavy ion collisions. These variables are very sensitive to the size and the density of the system formed in such collisions. The R_{CP} is expected to be less than unity if there is a creation of strongly interacting matter. In addition, it can show baryon-meson splitting at intermediate p_T region where quark recombination model is expected to be followed. If the heavy-ion collision is a simple super position of p+p collision, one would expect the value of R_{AA} to be unity. Any value of R_{AA} less than unity at high transverse momentum (p_T > 6 GeV/c) signifies the energy loss of the high p_T partons inside the hot and dense medium formed. In this thesis we will obtain the R_{CP} and R_{AA} of K*° to understand the partons energy loss in the hot and dense medium formed in high energy collisions. It will be compared with other particles to understand the baryon-meson effect at intermediate p_T.

The in-medium effects can also be studied through other observables like elliptic flow coefficient v_2. The v_2 of K^{*0} at low p_T could be modified due to the effect of hadronic re-scattering. In this thesis, we will present the measurement of v_2 of K*° in non-central Pb+Pb collisions at ^/s_{NN} = 2.76 TeV. The v_2 will be compared with that of other particles.

The high momentum heavy resonances can be used to look for the in-medium effects through the study of correlation with respect to a jet or a leading particle. The resonance-jet correlation in the same side and away side can distinguish between in-medium and in-vacuum fragmentation by assuming that the same side resonance properties and production remain unaffected due to surface bias, whereas the away side of the resonances are likely interacting with the hot and dense partonic medium. The enhanced cross-section of jets at LHC energies make such study more promising and interesting. In this thesis, we will present the study of K*°-jet correlation in p+p collisions at ɣ/s = 7 TeV. We will study the mass, width and yield of K*° with respect to the leading particle. This analysis will be a baseline for the future study in Pb+Pb collisions.

The second part of the thesis deals with the production mechanism of another identified particle, the photons. A Photon Multiplicity Detector (PMD) was build and installed at the LHC to provide the photon multiplicity and pseudo-rapidity distribution at forward rapidity (2.3 < q < 3.9). The photon measurement provides a complimentary information to that of charged pions as majority of photons are the decay of neutral pions. Such a measurement extends our knowledge of particle production to forward rapidities where one enters into a regime of small Bjorken x, in which gluon saturation is expected to occur. In this thesis, we have developed a technique of unfolding for PMD which is used for correcting the detector acceptance and efficiency. We will present the multiplicity and pseudo-rapidity distribution of photons at 2.3 < q < 3.9 in p+p collisions at ɣ/s = 900 GeV. To understand the particle production mechanism in different rapidity regions, we will compare our photon results at forward rapidity to that of charged particles at

mid-rapidity. We will also compare the results with the expectation from various models like PYTHIA and PHOJET. These results will also be used to study the limiting fragmentation behaviour at LHC energies.

Finally we will discuss through a phenomenological study of the production of identified baryons (specifically protons and anti-protons) in proton-proton collisions at high energy. The study of anti-proton to proton ratio (p/p) provides a valuable information to the production mechanism of baryons. In this thesis, we will present the results of p/p ratio in p+p collisions at various beam energies (23 GeV to 7 TeV) using different models PYTHIA, PHOJET and HIJING-BB. We will compare our results of p/p ratio from various models with the available experimental data to understand the mechanism of baryon production and baryon stopping at mid-rapidity in p+p collisions.

Publications

1. K*(892)^0 and 0(1020) production in Pb-Pb collisions at ^{p}SNN = 2.76 TeV *
   ALICE Collaboration (B. Abelev et al.), e-Print: arXiv:1404.0495v1 [nucl-ex], (Submitted to Phys. Rev. C)
2. Production of K*(892)^0 and 0(1020) in pp collisions at pS = 7 TeV *
   ALICE Collaboration (B. Abelev et al.), Eur. Phys. J. C72 (2012) 2183, e- Print: arXiv:1208.5717 [nucl-ex]
3. Strange hadron and resonance production in Pb-Pb collisions at psNN = 2.76 TeV with ALICE experiment at LHC*
   Subhash Singha (for ALICE Collaboration), Nuclear Physics A904-905 (2013) 539c-542c e-Print: arXiv:1211.0187 [nucl-ex]
4. Hadronic resonance production with ALICE experiment at LHC*
   Subhash Singha (for ALICE Collaboration), Proceedings of science (CPOD 2013) 055 e-Print: arXiv:1306.0673 [nucl-ex]
5. Inclusive photon production at forward rapidities for proton-proton collisions at pS = 0.9, 2.76 and 7 TeV*
   Under ALICE Collaboration review. (Target journal Eur. Phys. J C)

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1. Energy dependence of anti-proton/proton ratio in p+p collisions*

Subhash Singha, P.K. Netrakanti, Lokesh Kumar and B. Mohanty, DAE symposium 2010, http:// www.sympnp. org / proceedings/55/F17.pdf

2. Unfolding method for obtaining the photon multiplicity distribution at forward pseudo-rapidity in high energy p+p collisions*

S.K.Prasad, Subhash Singha, B. Mohanty and S. Chattopadhyay, DAE symposium 2010, http:// www .sympnp. org/proceedings/55/G37.pdf

3. K*^{0} resonance production in Pb-Pb collisions at ^{p}SNN = 2.76 TeV*

Subhash Singha (for ALICE collaboration), DAE symposium 2012, http:// www.sympnp. org / proceedings/56/F9.pdf

4. Expectation of photon multiplicity in p-p collisions at LHC energies*

Subhash Singha, S. De, B. Mohanty and T.K. Nayak, DAE symposium 2012, http:// www.sympnp. org / proceedings/56/F45.pdf

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Title	:	Going Out of Equilibrium in ADS/CFT

Abstract

As of now, string theory is believed to be the most successful quantum theory of gravity and a strong contender to be the fundamental microscopic theory of "everything". It starts with the idea that the world at its microscopic-most level is made up of some tiny stringy objects, which vibrate, do all kinds of funny acts and finally come up with the macroscopic world we see everyday. The different vibrational modes give rise to different elementary particles which we had so far been thinking of as the fundamental constituents of the universe. In other words, the long term goal of string theory is to provide a complete and universal microscopic foundation to more macroscopic theories and phenomenologies, such as the standard model of particle physics and Einstein's theory of gravitation, to name a few. However, string theory is a framework that operates in such an ultra-high energy regime that this is far beyond the reach of even the most modern particle accelerators like RHIC and LHC. But this is not really a matter to worry as such. Asking whether string theory can explain the real world is probably as irrelevant as to ask whether one can solve the problem of the oscillation of a simple pendulum in quantum field theory. We need to remember, just like quantum field theory, the theory of strings is also a framework, the justification whereof would probably be found from the theories derived from it.
With this aim in view string theory has expanded its horizon to other branches of theoretical physics where the possibility of having a derived theory with greater testibility increases with a decrement in energy scale. AdS/CFT correspondence is one such hypothesis derived in the string framework that nurtures this possibility. AdS/CFT, as we would discuss in gory detail in due course, is an illustrative realization of the old holographic principle which states that the degrees of freedom of quantum gravity reside on the boundary space-time. This in turn gives rise to a duality principle that maps the states in gauge theory to solutions in string theory living in one higher dimension. Particular significance and predictibility of such a miraculous hypothesis can be put to test when the t'Hooft coupling and the rank of the gauge group of the gauge theory in question becomes so high that it becomes intractable by traditional methods in quantum field theory. Even in this case, the hypothesis ensures the "dual" theory to be a simple classical theory of gravity with minimally coupled matter fields, namely the supergravity theory that is also realized as some consistent trancation of string theory at low energy. The advantage of working in supergravity limit of string theory is that unlike the full string theory which is a theory with infinite degrees of freedom, here one has to deal with only finite degrees of freedom.

Publicaiaons

Anisotropic branes",

1. Souvik Banerjee, Samrat Bhowmick, Sudipta Mukherji Phys. Lett. B 726, 461 (2013) arXiv:1301.7194 [hep-th].
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A (*) indicates papers on which this thesis is based.

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Title	:	Study of Laser-Cluster Interaction in Gas Phase

Abstract

Interaction of different atomic [Xe_n] and molecular [$(CF_2Br_2)_n$, $(C_2H_5Br)_n$, $(CH_3I)_n$] clusters with nanosecond laser pulses of intensity ~ 10^9 W/cm^2 has been studied using time- of-flight mass spectrometry. The time-of-flight mass spectra displays multiply charged atomic ions with broad peaks, implying high kinetic energy of the ions. Generation of multiply charged atomic ions at laser intensity ~10^9 W/cm^2 is unusual and thus a systematic study has been carried out to understand laser-cluster interaction mechanism by varying different experimental parameters such as laser wavelength, laser intensity, laser polarisation, cluster size, cluster composition etc. Experimental results illustrate that charge state of atomic ions increases with increasing laser wavelength. However, laser intensity does not affect the charge state of atomic ions under gigawatt laser intensity conditions. A threshold cluster size was found to be essential for observation of multiply charged atomic ions. For studies carried out on doped clusters, multiply charged atomic ions of dopant molecule were also observed. Kinetic energy of the multiply charged ions was determined under different experimental conditions. Kinetic energy was found to increase with charge state of multiply charged atomic ions, cluster size and laser wavelength. Further, charge density at the laser-cluster interaction zone was also measured for different cluster system, at different laser wavelength. Charge density was found to increase with laser wavelength for different atomic/molecular cluster, indicating efficient laser-cluster interaction at longer wavelength leading to generation of higher charge states of atomic ions. The experimental results obtained in the present work have been rationalized based on a three stage cluster ionization model. According to the model, multiphoton ionisation of atoms/molecules of cluster is the initial ionisation process which gives rise to quasi-free electron within the cluster. These quasi-free electrons interact with the laser field and gain energy due to inverse bremsstrahlung process and cause multiply charged ions within the cluster due to electron impact ionisation. When the Coulombic forces overcome the cohesive energy of the cluster, cluster disintegrates violently. Based on the experimental results of the thesis, following conclusions are drawn - a) multiply charged atomic ions were observed in laser-cluster interaction at laser intensity as low as ~ 10^9 W/cm^2 b) longer laser wavelength was found to facilitate generation of higher charge state c) a threshold cluster size is essential for observation of multiple charge atomic ions.

Publications

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4. "Size and wavelength dependent photoionisation of Xenon clusters." S. Das, P. M. Badani, P. Sharma and R. K. Vatsa. Chemical Physics Letters 2012, 552, 13-19.
5. "Diverse photochemical behavior of dibromodifluoromethane (CF2Br2) monomer and cluster under gigawatt intensity laser fields." S. Das, P. M. Badani, P. Sharma and R. K. Vatsa. RSCAdvances 2013, 3, 12867-12873.
6. "Understanding laser-cluster interaction: A case study of methyl iodide clusters ionized by gigawatt intensity laser pulses." S. Das, P. Sharma, P.M. Badani and R. K. Vatsa. (Submitted)

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Title	:	Exploration of the Shell Effect on the Level Density Parameter Near Doubly Closed Shell Nucleus A~208

Abstract

The shell effect is manifested in finite fermionic systems such as atoms and nuclei and plays an important role in describing the structure and the properties of the matter. It also affects the nuclear level density, a fundamental property of the nuclei, which is defined as the number of nuclear energy levels per unit excitation energy. The nuclear level density makes a transition from the shell-dominated regime at low excitation energy to that of a classical liquid drop at high excitation. The damping of nuclear shell effect with excitation energy has been addressed experimentally by measuring neutron time of flight spectra using triton transfer-fusion reaction on ^{205}Tl and ^{181}Ta targets with ^{7}Li beam from the Mumbai Pelletron Linac facility. A large area (~1×1m^2) plastic scintillation detector array has been setup for the measurement of the fast neutron by time of flight technique and an efficient CsI(Tl) detector array consisting 8 detectors couples to Si-PIN diode for the signal readout has been used for measurement of the alpha particles by pulse shape discrimination technique. The allowed values of the physical parameters related to the damping of the shell effect and the nuclear level density have been inferred for the first time. A precise measurement of these parameters in heavy magic nuclei will have wide implication in the context of current research on the formation of super heavy elements and nuclear astrophysics.

Publications

1. Measurement of the Damping of the Nuclear Shell Effect in the Doubly Magic ^{208}Pb Region P. C. Rout, D. R. Chakrabarty, V. M. Datar, Suresh Kumar, E. T. Mirgule, A. Mitra, V. Nanal, S. P. Behera, V. Singh,Phys. Rev. Lett. 110, 062501 (2013).
2. A large area plastic scintillator detector array for fast neutron measurements P. C. Rout, D. R. Chakrabarty, V. M. Datar, Suresh Kumar, E. T. Mirgule, A. Mitra, V. Nanal, R. Kujur, Nucl. Instrum. Methods Phys. Res., Sect.A 598, 526 (2009).

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Title	:	Development of Cryogenic Bolometer for Neutrinoless Double Beta Decay in ^{124}Sn

Abstract

Neutrinoless double beta decay (0 is the only known process which can provide information)vββ) about the Majorana nature of the neutrinos and also enable the experimental measurement of the absolute mass scale of the (Majorana) neutrinos. In India, efforts have been initiated for experiment to look for 0vββ in 124Sn (Qββ=2.28 MeV, 5.8% abundance) at the upcoming underground facility of India Based Neutrino Observatory (INO). The identification of 0vββ necessarily relies on measurement of the sum energy (= Qββ) of the two emitted electrons and requires a high resolution detector to detect the 0vββ process in the presence of more probable 2vββ process. Cryogenic calorimetric particle detectors (bolometers) have excellent energy resolution and high sensitivity. The R&D related to the fabrication of a large size Tin (superconducting) cryogenic bolometer has been carried out as a part of this thesis work. This involved the design and performance optimization of CFDR-1200 dilution refrigerator for

bolometer studies at mK temperature. The CFDR-1200 has a high cooling power of 1.4 mW at 120 mK and has been successfully installed and tested at TIFR, Mumbai. The mixing chamber of the CFDR-1200 is capable of supporting and cooling 100 Kg weight and has a cylindrical sample space of 300 mm x 300 mm. The lowest minimum temperature of 7 mK was achieved without any external heat load on the system. The thesis also describes the procedure to measure the heat capacity of superconducting calorimeter absorbers below 100 mK along with results for Sn. A calorimeter set up has been devised to measure ultra small heat capacity of superconductors below 400 mK in the CFDR-1200. The heat capacity of Tin samples have been investigated to check if anomalous specific heat could affect the energy resolution of an energy calorimeter. The specific heat of Tin has been measured in the temperature range of 60 - 400 mK and the Debye temperature obtained (199±9 K) has been found to be consistent with the value reported in literature. The absence of anomalous heat capacity in the Tin sample at T<100 mK suggests that it should be possible to achieve a complete thermalization of energy in a Tin bolometer absorber. Also, no difference is found between the heat capacity of a polycrystal and a single crystal sample. Simulations have been carried out to optimize the detector element size for photon background reduction based on hit multiplicity. The possibility to use multiplicity (M) to discriminate between electron (M=1) and gamma rays (M>1) has been studied for various detector geometries. The results indicate that the element size of 3x3x3 cm3 is a preferable choice for the detector element from the calorimetry , granularity (limitation of readout sensors) and gamma ray background reduction capability. The optimal detector module design proposed consists of 27 elements of 3x3x3 cm3 each, arranged in a cubic array of 3x3x3 such that the central element is covered on all sides by other detector elements. The estimated detection efficiency of this module (mass 5 Kgs) is ~86% for 0νββ events. The modules can be arranged in a tower geometry for upscaling to large mass experiments in a phased manner.

Publications

A) Publications Arising from the Thesis

1. Heat capacity setup for superconducting bolometer absorbers below 400mK, V. Singh,Mathimalar. S, N. Dokania, V. Nanal, R. G. Pillay, S. Ramakrishnan, Journal of Lowtemperature Physics 175 (2014) 604.
2. Cryogen Free Dilution Refrigerator for bolometric search of neutrinoless double decay(0___) in 124Sn, V. Singh, Mathimalar. S, N. Dokania, V. Nanal, R. G. Pillay, S.Ramakrishnan, Pramana - Journal of Physics 81 (2013) 719.
3. Simulation studies for the Tin Bolometer Array for Neutrinoless Double Beta Decay, V.Singh, Mathimalar. S, N. Dokania, V. Nanal, R. G. Pillay, paper submitted to Pramana-Journal of Physics.

B) Conference Papers

1. Development of Cryogenic Bolometer for 0___ in 124Sn, V. Singh, G. Yashwant, S. Mathimalar,Neha Dokania, V. Nanal, R. G. Pillay, V. M. Datar, AIP Conf. Proc. 1405, pp.334-336 (2011).
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C) Others

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Title	:	Dislocation Dynamics Simulations of Strain Localization in Irradiated Steels

Abstract

Dislocation-Dynamics (DD) refers to a mesoseale simulation and modelling tool for understanding dislocation mediated phenomena, using the mobility rules obtained from the lower scale simulation techniques like molecular dynamics. This thesis employs the DD technique to understand the following issues:

1, The evolution of dislocation microstructure in ferritic steels in presence of irradiation induced prismatic loops and oxide-dispersions,
2, Understanding the role of stresses on the primary and cross-slip planes on the features of multiple clear channels formed in austenitic stainless steels,
3, Study the variation of the equilibrium stacking fault width of a split FE source under the simultaneous application of glide and Escaig stresses acting in its glide plane. And also to understand the role of glide and Escaig stresses acting on the primary and cross-slip planes in the cross-slip of a pinned screw dislocation.

These simulations required adding new computation modules and post-processing tools to the existing DD packages. Significant observations coming out of the present thesis are as follows:

1, It was found that cross-slip is a important factor that controls the strain localization. In ease of irradiated ODS steels, the Orowan loops formed around the dispersoids due to the dislocation glide, enhance the cross-slip probability and hence provide greater strain spreading than in irradiated steel devoid of these dispersoids,
2, In studies of clear channel formation in fee, it was found that the separation of clear channels is function of the grain size, irradiation dose as well as the stacking fault energy.

It is also shown that the stress held developing in the vicinity of a clear band can be described through a simple analytical expression accounting for the applied stress magnitude, the grain size and the critical cross-slip stress,

3, Through the nodal based DD simulations of split FE sources, it was found that the presence of Escaig stresses directly affects the equilibrium dissociation width, and hence impacts the cross-slip probability of a screw dislocation,

4, Under the application of stress tensors of a certain form, it is found that the behavior of the screw dislocations with constrictions is different if the dislocation segments are composed of partial segments than perfect segments. The propensity for the cross-slipped segment to spread over its full length is seen predominantly dependent on the glide stresses acting on the primary and cross-slip planes.

Publications

1. Plastic deformation of ferritic grains in presence of ODS particles and irradiation- induced defect clusters: A 3D dislocation dynamics simulation study
   C. Robertson, K. Gururaj Journal of Nuclear Materials 415 (2011) 167-178.
2. Plastic Deformation in ODS Ferritic Alloys: A 3D Dislocation Dynamics Investigation
   K. Gururaj, C. Robertson Energy Procedia 7 (2011) 279-285.
3. Channel formation in irradiated FCC metals: a 3D dislocation dynamics investigation
   K. Gururaj, C. Robertson, M. Fivel Phil Mag (Referee comments recieved)
4. Post-irradiation plastic deformation in bcc Fe grains investigated by means of 3D dislocation dynamics simulations
   K. Gururaj, C. Robertson, M. Fivel Journal of Nuclear Materials (communicated)

Manuscripts to be communicated

1. Role of Schmid and Escaig stresses in the evolution of Split Frank-Read sources:
   A dislocation dynamics study
2. Dynamics of a Frank-Read source with constrictions: A nodal based dislocation- dynamics simulation.

Publications not part of the thesis

1. Confomational and coalescence behavior of Trialkylphosphates in various diluents
   A.S. Suneesh, G.V.S, Ashok Kumar, K. Gururaj, K.A. Venkatesan, M.C. Valsa Kumar, P. R. Vasudeva Rao.
   Journal of Molecular Modelling (2014) 20, 1-8.
2. Computation of thermal conductivity: A nonequilibrium approach P. Anees, K. Gururaj and M. C. Valsakumar.
   AIP Conf. Proc. 1447, 1011 (2012)
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   Applied Surface Science 255 (2008) 104.

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Title	:	Ab inito Studies on Properties of Nanostructures

Abstract

Mr. C. Kamal has carried out computational studies on the properties of nanostructures namely, graphene-like honeycomb structures, carbon and gallium phosphide nanotubes, gallium phosphide and aluminium phosphide clusters, and homonuclear diatomic molecules by employing density functional theory / time dependent density functional theory based calculations. Some of the salient features of his work are given below.

Geometric and electronic structure calculations of both mono-layer and multi-layer of graphene-like honeycomb structure - silicene have been performed. The calculations of monolayer of silicene predict that there is a possibility of opening up of a tunable band gap in silicene due to a transverse static electric field. In case of multi-layers, presence of strong covalent bonds between the layers of silicene multi-layers is observed. This covalent nature of the bonds is different from the weak van der Waal's interaction between the layers of graphene multi-layers. It has been shown that the presence of strong covalent bonds significantly influences the properties of multi-layers. The studies on carbon and gallium phosphide nanotubes show that both these two nanotubes are semiconductors with direct band gaps, unlike their bulk counterparts which have indirect band gaps. It is also observed that there is a semiconductor to half-metallic/metallic transition due to intercalation of alkali and transition metal atoms in these nanotubes. The evolution of optical response properties of carbon nanostructures such as carbon nanotubes and fullerenes as a function of their sizes has been studied. Calculations predict the presence of a large anisotropy in the polarizability of carbon nanotubes which is likely to play an important role in electric field assisted oriented growth of carbon nanotubes. The calculations of van der Waals interaction coefficient predict that there is a strong interaction between the carbon nanostructures and environmentally important gases namely green-house and toxic gases. Studies on evolution of static polarizability of lll-V clusters such as GaP and AIP, with the size of clusters have been carried out. The calculations predict that the values of polarizability of these clusters decrease with increasing size and reach their limit from above. A detailed investigation on the effect of different exchange-correlation functionals on the static polarizability of GaP clusters has also been carried out. The studies on various homonuclear diatomic molecules show that many physical and chemical properties of these diatomic molecules show periodic variation along the rows/columns of periodic table.

Publications

1. Ab initio Study Of Stoichiometric Gallium Phosphide Clusters C. Kamal, Tapan K. Ghanty, Arup Banerjee, and Aparna Chakrabarti Journal of Chemical Physics, 130, 024308 (2009)
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3. Interesting Periodic Variations In Physical And Chemical Properties Of Homonuclear Diatomic Molecules C. Kamal, Arup Banerjee, Tapan K. Ghanty, and Aparna Chakrabarti International Journal of Quantum Chemistry, 112, 1097 (2012)
4. Silicene Beyond Mono-layers - Different Stacking Configurations And Their Properties C. Kamal, Aparna Chakrabarti, Arup Banerjee, S. K. Deb Journal of Physics: Condensed Matter, 25, 085508 (2013)
5. Ab initio Studies Of Effect Of Intercalation On The Properties Of Single Walled Carbon And Gallium Phosphide Nanotube C. Kamal, Aparna Chakrabarti, Arup Banerjee, S. K. Deb

Physica E: Low-dimensional Systems and Nanostructures, 54, 273 (2013)
Ab initio Investigation On Hybrid Graphite-like Structure Made Up Of Silicene And Boron Nitride C. Kamal, Aparna Chakrabarti, Arup Banerjee Physics Letters A, 378, 1162 (2014)

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1. Properties Of Two-Dimensional Silicon Versus Carbon Systems C. Kamal, Arup Banerjee, and Aparna Chakrabarti Graphene Science Handbook: Size-Dependent Properties, CRC Press, Taylor & Francis Group (Invited, submitted)

In Conferences

1. Properties of Multi-layered and Hybrid Structures of Silicene : A Detailed DFT Study C. Kamal (Invited) International Conference Superstripes 2014, Ettore Majorana Foundation and Centre for Scientific Culture, Sicily, ITALY (25-31 July 2014).
2. Computational Studies On Two Dimensional Graphene-like Structures C. Kamal (Invited) Workshop on Advances in Computational Physics (ACP2013), Central University of Tamil Nadu, Thiruvarur, INDIA (14-16 February 2013).
3. Ab initio Studies On Properties Of Graphene-like Honeycomb Structures C. Kamal, Aparna Chakrabarti, Arup Banerjee and S. K. Deb An Advanced School On Modeling Transition Metal Oxides (ATHENA-2012), S. N. Bose National Centre for Basic Sciences, Kolkata, INDIA (09 - 12 Apr, 2012) The van der Waals Interaction Between Diatomic Molecules C. Kamal, Arup Banerjee, Tapan K. Ghanty and Aparna Chakrabarti Topical Conference on Interaction of EM Radiation with Atoms, Molecules and Clusters (TC -2010), Raja Ramanna Centre for Advanced Technology, Indore, INDIA (03 - 06 Mar, 2010)
4. Electronic Structures Of Transition Metal Doped Group IV And III-V Nanotubes Aparna Chakrabarti and C. Kamal Psi-K conference 2010, Henry Ford Building, Fritz Haber Institut der Max Planck Gesellschaft, Berlin, GERMANY (1 2 - 1 6 Sep, 2010)
5. The van der Waals Interaction Between Carbon Nanotubes, Fullerenes And Small Molecules C. Kamal, Tapan K. Ghanty, Arup Banerjee, and Aparna Chakrabarti International Conference on Materials for Advanced Technologies (ICMAT 2009), Symposium H: Carbon nanotubes: Synthesis, Characterization and Applications, Suntec Singapore International Convention & Exhibition Centre, SINGAPORE (28 Jun - 03 Jul, 2009)

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Title	:	Wireless Sensor Networks for Nuclear Reactor Applications

Abstract

Wireless Sensor Networks is an emerging technology and research is inprogress to use this powerful technology in industrial and other areas for process monitoring, military surveillance, environmental monitoring, structural health monitoring, health monitoring etc. The Wireless Sensor Networks (WSN) have many advantages over wired networks. In WSNs there are no cables for transmission of data. Hence the cable cost and cabling cost will not be there. Also there are no fire risks associated with cables. WSNs permit automatic reconfiguration thus providing redundant path even an in between routing node fails. Thus WSNs will reduce capital costs and improve the safety depending on the application. However there are many challenges to be overcome such as limited processing power, limited battery life, security etc. Also there is no literature which indicates that wireless sensor networks have been used extensively for process monitoring in nuclear reactors and it's facilities. As the advantages outweigh the challenges, it was decided to work on this technology and make robust and reliable networks for process monitoring in nuclear reactors and it's facilities which will be acceptable to the nuclear

regulators.

The thesis explains the research and development work that is carried in this domain of wireless sensor networks for using them in Nuclear Reactor applications for process monitoring. The thesis work covers the advantages, challenges, various applications, architecture of the node, commercial nodes available in the market, WSN standards, protocols etc. It covers the motivation for research, scope of research, the signal penetration studies in hot cells and reactor containment building, the research & developmental works carried out to develop different types of nodes for various applications, development of software stack etc. It explains the various deployments in the WSN lab and for temperature and humidity monitoring of high performance computer cluster facility. It also explains different and varied types of wireless sensor network deployments in nuclear reactor field viz. radiation monitoring in radio chemistry laboratory, in sodium test facility, safety grade decay heat removal loop, and in fast breeder test reactor The implementation of security protocol to improve the security along with it's overhead study is narrated. The networks have been monitored and successful performance was observed over a long time to give the confidence to the designers and nuclear regulators. The development of wireless network management system to get the topology view and trend view of the parameters being monitored is explained.

The performance of the network with respect to through put analysis, packet drop ratio is also measured and analyzed and found to be satisfactory.

Publications

1. Wireless Sensor Network in Fast Breeder Teat Reactor, S.A.V. Satya Murty, Baldev Raj, Krishna M. Sivalingam, S.Sridhar, Jemimah Ebenezer, Kalyan Rao Kuchipudi Journal of Nuclear Engineering & Technology 3 (2013) 28-36
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3. Experimental Deployment of Wireless Sensor Network for Radiation Monitoring S.A.V. Satya Murty, Baldev Raj, Krishna M. Sivalingam, Jemimah Ebenezer, R. Parthasarathy, D. SaiSubalakshmi, Journal of Nuclear Engineering & Technology 2 (2012) 10-21

Conference Publications International

1. Real Time Routing Protocols for Wireless Sensor Networks : A Survey Pradeep Chennakesavula, Jemimah Ebenezer, S.A.V. Satya Murty Fourth International Conference on Wireless and Mobile Networks (WiMo-2012) at Avinasalingam University, Coimbatore Oct 26-28, 2012.
2. Experimental Analysis of RSSI for Distance and Position Estimation Vinita Daiya, Jemimah Ebenezer, S.A.V. Satya Murty, Baldev Raj International Conference on Recent Trends in Information Technology (ICRTIT) at MIT, Chennai, June 2011.
3. Low Latency and Energy Efficient Routing Protocols for Wireless Sensor Networks D. Baghyalakshmi, Jemimah Ebenezer, S.A.V. Satya Murty International Conference on Wireless Communication and Sensor Computing [ICWCSC] at SSN College of Engg, Chennai, Jan 2010
4. Low Latency Energy efficient MAC protocols for Wireless Sensor Networks G. Sandhya Rani, Jemimah Ebenezer, S.A.V. Satya Murty International Conference on Sensors and Related Networks at VIT University, Vellore, Dec 7-10, 2009
5. Architecture for Real Time Communication in Wireless Sensor Networks D. Baghyalakshmi, Jemimah Ebenezer, S.A.V. Satya Murty International Conference on Sensors and Related Networks at VIT University, Vellore. Dec 7-10, 2009
6. Security issues in Wireless Sensors Networks S. A.V. Satya Murty (invited presentation) International Conference on Sensors and Related Networks (SENNET-07) at VIT University, Vellore, Dec 12-14, 2007.
7. Wireless Sensor Networks: Security Concerns S.A.V. Satya Murty (invited presentation) In pre conference tutorial of International Conference on Sensors and Related Networks (SENNET-07) at VIT University, Vellore, Dec 10-11, 2007.

National

1. Wireless Sensor Networks for Process Monitoring in Power Plants S.A.V. Satya Murty (invited presentation) National Workshop on Sensors for Power Plant process & Equipment by NTPC at Noida, 21st June 2013
2. Wireless Sensor Networks in Nuclear Facilities S.A.V.Satya Murty (invited presentation) BRNS theme Meeting on Electronics and Security at BARC, Mumbai, 27th Feb, 2013
3. Wireless Sensor Networks: The Emerging Technology S. A.V. Satya Murty (invited presentation) Theme meeting on Novel and Innovative Measurements in Non Destructive Evaluation, Feb 23-24, 2012.
4. Deployment Challenges of Wireless Sensor Network for Nuclear Applications Jemimah Ebenezer, D.Baghyalakshmi, G. Sandhya Rani, S.A.V. Satya Murty Sangoshthi-2012, BHAVINI, Kalpakkam, Dec 21-23, 2012
5. Management Issues of Wireless Sensor Networks T. S. Shrikrishnan, Sukant Kothari, Jemimah Ebenezer, K. Kuriakose, S.A.V. Satya Murty Sangoshthi-2012, BHAVINI, Kalpakkam, Dec 21-23, 2012
6. Study on Effect of Radiation Shield RCB Wall on RF Signal Vinita Daiya, Jemimah Ebenezer, K. Kuriakose, S.A.V. Satya Murty Sangoshthi-2012, BHAVINI, Kalpakkam, Dec 21-23, 2012
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8. Test bed based Throughput Analysis in a Wireless Sensor Network Anand Kumar, P. Gireesan Namboothiri, Sarang Deshpande, Sreejith Vidhyadharan, Krishna M. Sivalingam, S.A.V. Satya Murty National Conference on Communications (NCC), Kharagpur, Feb. 2012.
9. Wireless Sensor Networks and its Applications S.A.V. Satya Murty Theme Meeting on Instrumentation for Nuclear Facilities at IGCAR, Kalpakkam, 30th Dec 2008.

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Abstract

The India-based Neutrino Observatory (INO) will host a 50 kt magnetized iron calorimeter for the study of atmospheric neutrinos, which will have a modular structure of dimension 49m X 16m X 14.5m and will consist of a stack of 150 horizontal layers of 5.6 cm thick magnetized iron plates interleaved with 2.5 cm gaps to house the active detector layers. The ICAL detector will be subdivided into three modules of the dimension 16.2m X 16m X 14.5m. As active element ICAL will use Resistive Plate Chambers(RPC), whose readout will be performed by external orthogonal pickup strips of 3cm width. Being magnetized, ICAL will have charge identification capability, which in turn will help in determining the true mass hierarchy (MH) of neutrino, depending on the fact that the event rate will be different for neutrinos and antineutrinos due to the matter effect. Apart from determining the true MH, INO has set the precise measurement of atmospheric mass difference and atmospheric mixing angle as its major goal. The atmospheric muon neutrinos, interacting with the detector, generates the muon associated with a hadron shower. The muon gives a clear track inside the detector, while the hadrons interacting with the iron plate generate the shower, producing a bunch of hits in RPCs. To reconstruct the neutrino energy, it is essential to reconstruct the muon and hadron energy both. From the track, the muon momentums are reconstructed using both tracklength and curvature method. From the hit distribution of the hadrons, the energy of the hadrons are calibrated.

In this thesis, I presented results from the study of the behaviour of hadrons inside ICAL. In

particular, I showed the hadron energy resolution of ICAL which was obtained using the Geant4 as simulation tool for the ICAL detector. As part of my PhD work, I studied the MH sensitivity of this experiment, using data simulated with a Nuance based event generator developed for ICAL, and folded with the detector resolution and efficiencies obtained by the INO collaboration from a full detector Geant4 based simulation. The ICAL data was combined with data from T2K, NOnA, RENO, DayaBay and DoubleChooz experiments which were simulated using GLOBES package, and their combined sensitivity to the MH was studied. To satisfy the constant pursuit of improving the potential of atmospheric experiment in MH measurement, we included the hadron events in the analysis, by tagging them with zenith angle of the corresponding muon, produced in the charge current interaction of the neutrino, and binning the hadron data first in energy and then in zenith angle. A combined statistical analysis, including muon and hadron events, showed that the addition of hadron data into the analysis improve the MH sensitivity even further. Finally, I showed the potential of ICAL in measuring the atmospheric mass square difference and atmospheric mixing angle precisely.

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5. Anushree Ghosh, Sandhya Choubey, Measuring the Mass Hierarchy with Muon and Hadron Events in Atmospheric Neutrino Experiments, JHEP 1310, (2013), 174 .
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7. Moon Moon Devi, Anushree Ghosh, Daljit Kaur, Laksmi Mohan, S. Choubey, A. Dighe, D. Indumathi, S. Kumar, M. V. N. Murthy, Md. Naimuddin, Hadron energy resolution as a function of iron plate thickness at ICAL, JINST 9 (2014) 09, T09003 .

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Abstract

The thesis reports design and development of experimental facilities viz.(confocal micro Raman scattering setup and Energy dispersive/Angle dispersive X-ray diffraction beamline) for high pressure measurements and detailed investigations of structural behaviour of some geophysical materials under high pressure using x-ray diffraction, Raman spectroscopic and simulation techniques.

The designed confocal micro Raman setup helps in recording the signal from weak scatterer inside DAC. The beamline provide the capability of investigating the materials under high pressure using synchrotron based energy dispersive/angle dispersive x-ray diffraction measurements. It is also adapted for high pressure single crystal diffraction measurements.

High pressure investigation on cristobalite form of AlPO4 using Raman scattering, x-ray diffraction and simulations (classical as well as first principles calculations) show that the high pressure behavior of c-AlPO4 significantly depends on the extent of non-hydrostatic stresses. In non-hydrostatic conditions, it transforms at very low pressure ~2 GPa to monoclinic phase which on further compression leads it to transform to the Cmcm phase. In hydrostatic conditions ambient c-AlPO4 directly transforms to the Cmcm phase. The transformation mechanism is studied using classical and first principles simulations.

The high pressure behavior of several silica analogs viz. AlPO4, GaPO4, InPO4, FePO4, and BPO4 have also been studied using first principles calculations in high pressure region to investigate the mechanism of formation of six coordinated phosphorous as the high pressure phase of AlPO4 and GaPO4 (i.e. the Cmcm phase) is further compressed. It is shown that smaller cations favor six-coordinated denser phase at low pressures, compared to the Cmcm phase. These calculations suggest that six coordinated phase in $FePO_4$ can be realized at pressures as low as ~25 GPa.

Hydrous magnesium silicates Phase-A and super hydrous phase-B (Shy-B) have been investigated for structural stability using first principles simulations. These materials are assume to be a major source of the water reservoir in the deep interior of the Earth. The investigations show as to how an increase in the non-bonded H- - -H repulsion energy due to compression is relieved. The results show that it happens by cooperative distortion of full geometry of the hydrogen bond.

Publications

International Journal

1. High pressure investigations on hydrous magnesium silicate-phase A using first principles calculations H---H repulsion and changes in hydrogen bond geometry with compression; Authors- H.K. Poswal, Surinder M. Sharma and S.K. Sikka; (High Pressure Research, 29, 405,(2009))
2. Investigation of structure and hydrogen bonding of superhydrous phase B (HT) under pressure using first-principles density functional calculations; Authors- H. K. Poswal; Surinder M. Sharma; S. K. Sikka; (High Pressure Research, 30, 198, (2010))
3. Pressure-induced structural transformations in the low-cristobalite form of $AlPO_4$ Authors H.K. Poswal, Nandini Garg, Maddury Somayazulu, and Surinder M. Sharma (American Mineralogist, 98, 285–291,(2013))
4. Energy dispersive x-ray diffraction beam line at Indus-2 Synchrotron source K.K. Pandey, H.K. Poswal, A.K. Mishra, Abhilash Dwivedi, R. Vasanthi, Nandini Garg and Surinder M. Sharma (Pramana J. Physics, 80,607-619,(2013))
5. Pressure Induced Structural Transformation of the low cristobalite form of $AlPO_4$ Investigated by First Principles Calculations H. K. Poswal and Surninder M. Sharma

(Submitted)

6. Study of six coordinate phosphorus by oxygen under pressure using first principles calculations H. K. Poswal, Surninder M. Sharama (Manuscript prepared)

Symposium Papers:

1. High pressure investigations on Dense Hydrous Magnesium Silicate (Phase A) using first principles calculations Authors- H. K. Poswal, Surinder M Sharma and S. K. Sikka (Proceedings of the DAE Solid State Physics Symposium, 2008)
2. First principles investigations of pressure induced changes in hydrogen bonding in super-hydrous phase B; Authors- H. K. Poswal, Surinder M Sharma and S. K. Sikka Proceedings of the 54th DAE Solid State Physics Symposium (2009)

3. High pressure investigations on cristobalite form of AlPO4 Authors- H. K. Poswal, Nandini Garg, Maddury Somayazulu, Surinder M. Sharma, International Conference on High Pressure Science and Technology, AIRAPT-23, 181 (2011)
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5. Study of six coordinate phosphorus by oxygen under pressure using first principles Authors- H. K. Powal and Surnider M. Sharma (4^{th} interdisciplinary Symposium on Material Chemistry,2012)
6. First principles calculation on cristobalite form of AlPO4 Authors-H.K. Poswal and Surinder M. Sharma
   Solid state physics symposium, (2012)

Publications other than included in thesis

International Journal

7. Pressure Induced Structural Transformation in Silicon Nanowires Authors- H. K. Poswal, Nandini Garg, Surinder M. Sharma, E. Bussetto, S. K. Sikka, Gautam Gundiah, F. L. Deepak and Prof. C. N. R. Rao (Journal on Nanoscience and Nanotechnology, 5,729(2005))
8. Nature of Vn+ ions in SnO2: EPR and photoluminescence studies Authors- R.S.Ningthoujam, D. Lahiri, V. Sudarsan, H.K.Poswal, , S.K. Kulshreshtha, , S.M. Sharma, B. Bhushan, M.D.Sastry, (Materials Research Bulletin 42, 1293, (2007))
9. High Pressure behaviour of Ni-filled and Fe-filled multi-walled carbon nanotubes Authors- H. K. Poswal, S. Karmakar, P. K. Tyagi, D. S. Misra, E. Busetto, Surinder M. Sharma and A. K. Sood, (Physica Satus Solidi (B), 244 (10), 3612 (2007))
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11. Pressure induced structural phase transition in triglycine sulfate and triglycine selenateAuthrs- Rajul Ranjan Choudhury, H. K. Poswal, R. Chitra, Surinder M. Sharma, (The Journal of Chemical Physics 127, 154712, (2007)

12. Anomalous high pressure behaviour in nanosized rare earth sesquioxides Authrs-Nita Dilawar, Deepak Varandani, Shalini Mehrotra, H K Poswal, Surinder M Sharma and Ashis K Bandyopadhyay, (Nanotechnology, 19, 115703, (2008))
13. Structural Phase Transitions in $Zn(CN)_2$ under High Pressure Authors- H. K. Poswal, A.K. Tyagi, Andrea Lausi, S.K. Deb and Surinder M Sharma, (Journal of Solid State Chemistry; 182, 136, (2009))
14. Low-temperature and high-pressure Raman and x-ray studies of pyrochlore Tb2Ti2O7 Phonon anomalies and possible phase transition; Authors- Surajit Saha, D. V. S Muthu, Surjeet Singh, B. Dkhil, R. Suryanarayanan, G. Dhalenne, H. K. Poswal, S. Karmakar, Surinder M. Sharma, A. Revcolevschi, and A. K. Sood; (Physical Review B, 79, (2009) 134112)
15. Structural evolution of double perovskite Sr_2MgWO_6 under high pressure; Authors- A. K. Mishra, H. K. Poswal, S. N. Acharya, A. K. Tyagi, and S. M. Sharma; (Phys. Status Solidi B 247(7), 1773, (2010))
16. Pressure-induced anomalous phase transformation in nano-crystalline dysprosium sesquioxide; Authors- N. D. Sharma, J.Singh,S. Dogra, D. Varandani, H. K.Poswal, S. M. Sharma, A. K. Bandyopadhyay, (J. Raman Spectroscopy, 42, 438, (2011))
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18. First principles calculations on the effect of pressure on $SiH_4(H_2)_2$ Authors- K. V. Shanavas, H. K. Poswal and Surninder M. Sharma (Solid State Communications 152, 873-877 (2012))

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20. Pressure induced phase transitions in multiferroic $BiFeO_3$ Authors- A.K. Mishra; K.V. Shanavas; H.K. Poswal; B.P. Mandal; Nandini Garg; Surinder M Sharma (Solid State Communications, 154, 72-76, (January 2013))
21. High pressure iso-structural phase transition in $BiMn_2O_5$ Authors: K. K. Pandey, H. K. Poswal, Ravi Kumar and Surinder M. Sharma (Journal of Physics : Condensed matter, 25 ,325401, (2013))

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3. Behaviour of Ni-filled multiwall carbon nanotubes under high pressures Authors- H. K. Poswal, Pawan K. Tyagi, D.S. Misra, Surinder M Sharma and Ajay K. Sood, (Proceedings of the DAE Solid State Physics Symposium, 2006)
4. High pressure behavior of rare earth scandate Authors- Nandini Garg, H. K. Poswal, A. K. Tyagi and Surinder M. Sharma (Proceedings of the DAE Solid State Physics Symposium 51,157, 2006)
5. High pressure investigation of triglycine sulfate and triglycine selenate using Raman scattering and ab-inition calculations Authors- H. K. Poswal, Rajul Ranjan Choudhury, R. Chitra, Surinder M. Sharma, (ICAM 2007, Bangalore)
6. High Pressure Angle dispersive x-ray diffraction study of $Zn(CN)_2$ mAuthors- H. K. Poswal, A. K. Tyagi, S. K. Deb and S. M. Sharma Proceedings of the DAE Solid State Physics Symposium, 2007)
7. In-situ non-hydrostatic high pressure x-ray diffraction study of HgI_2 Authors: K.K.Pandey, H. K. Poswal and Surinder M. Sharma (DAE Solid State Physics Symposium Proceedings, 52, 175, 2007
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9. High Pressure Investigations of Glycinium Maleate; K. K. Pandey, Chitra Murli, Nandini Garg, H K Poswal, R Chitra and Surinder M Sharma; (Proceedings of the 53rd DAE Solid state Physics Symposium 267 (2008))
10. Structural study of double perovskite Sr_2MgWO_6; (AIP Conference Proceedings, 1313, 367, (2010))
11. First principles calculations on the effect of pressure on $SiH_4(H_2)_2$ Authors: K. V. Shanavas, H. K. Poswal, Surinder M. Sharma, (International Conference on High Pressure Science and Technology, AIRAPT-23, 249 (2011))
12. Behaviour of NTE material $Ag_3[Co(CN)_6]$ under pressure, Authors: Pallavi Ghalsasi, Ravi Tripathi, H. K. Poswal and Surninder M. Sharma, (International Conference on High Pressure Science and Technology, AIRAPT-23, 266 (2011))
13. Behaviour of NTE material Ag 3[Co(CN) 6] under pressure Authors- P. Ghalsasi, H.K. Poswal, R.Tripathi,N. Garg, M.N.Deo, Surinder M. Sharma (Journal of Physics: Conference Series, 377,(2013))
14. High pressure behavior of BiMn2O5 Authors- K.K. Pandey,H.K. Poswal, R. Kumar, Surinder M. Sharma (AIP Conference Proceedings, 1512,100-101)

15. Structural behaviour of Mg, Al and Si doped niobium oxynitrides under high pressures Authors- B.B. Sharma, H.K. Poswal, Surinder M. Sharma, J.V. Yakhmi, Y. Ohashi, S. Kikkawa (AIP Conference Proceedings, 1512, 108-109)
16. In-situ study of the growth of CuO nanowires by energy dispersive X-ray diffractionAuthors- H. Srivastava, T. Ganguli, S.K.Deb, T. Sant, H.K. Poswal, Surnider M. Sharma (AIP Conference Proceedings,1512, 306-307)

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Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	Systems Biology from Cell to Society: Transmission Dynamics in Complex Networks with Mesoscopic Organizatio

Abstract

With the completion of human genome mapping, the focus of scientists seeking to explain the biological complexity of living systems has gradually shifted towards understanding how the interactions amongst the large number of components result in the different functions of an organism. To this end, the area of systems biology attempts to achieve an integrated description of living processes by investigating the complex network of interactions between the various elements of different biological systems. Such networks are observed at many different length scales in the biological world, from protein contact networks at the molecular level to food webs observed at the level of an entire ecosystem. Thus, networks provide an unifying framework for understanding the operation of complex biological systems.

In this thesis, the results of theoretical and simulation studies exploring dynamical aspects of biological networks associated with host-pathogen interactions, that occur at the micro-scale (intra-cellular signaling networks), as well as, at the macro-scale (the contact network through which epidemics propagate in human societies) are described. At the intra-cellular scale, we have investigated the role of branched module motifs in the dynamics of Mitogen-Activated Protein Kinase (MAPK) signaling cascades. We demonstrate that the enzyme-substrate dynamics on branched structures allow surprisingly long-range communication across the network through retrograde propagation in the absence of any direct interactions between molecules in different branches of MAPK pathways. This can have potential significance in designing drugs targeting key molecules that regulate multiple pathways implicated in systems-level diseases such as cancer and diabetes. Also at the intra-cellular scale, we have explored the human cancer disease-gene network at the mesoscopic level. Our analysis of the functional roles of cancer genes using information about their intra- and inter- modular connectivity has revealed that 36 genes in the network act as “connector hubs”. The importance of these genes in cancer, which mark them as potential targets for therapeutic efforts, have been confirmed by correlating their occurrence in various human signaling pathways related to cancer, as well as, with data on survival rates of different cancers.

To understand disease dynamics at the macro-scale, we have analyzed the transmission patterns of the 2009 A(H1N1) influenza outbreak in India. Using a variety of statistical fitting procedures, we have provided a robust estimate of the basic reproduction number R_0 for the disease to be around 1.45 for India, a value which lies towards the lower end of the range of values reported for different countries affected by the pandemic. In the theoretical front, we have investigated the role of community organization in contact networks in the long-term dynamics of an epidemic. Our results for the SIRS (Susceptible-Infected-Recovered-Susceptible) epidemic model dynamics in modular networks suggest that, under certain circumstances, an epidemic can become persistently recurrent in a population. In particular, we have shown that highly

contagious diseases (large R_0), which quickly die out in a population with homogeneous contact structure, can survive indefinitely (becoming endemic) when there is strong community organization in the population. We have also explored the role of spatial geography in the spatio-temporal patterns of incidence of malaria in a region of northern Bengal. By subjecting the time-series data of malaria incidence (for both Plasmodium vivax and Plasmodium falciparum) from 51 different health centers in the region to wavelet phase analysis, we have identified epicenters of the disease from where they spread out to rest of the region. We have demonstrated a strong connection between the periodicity of malaria incidence and temporal variations in rainfall, which is established by simulations of a spatially detailed network model of malaria transmission. Our results can potentially be used to identify the key locations and periods for a focused vector eradication program in order to control malaria.

Thus, the results described in the thesis can potentially provide valuable inputs for pharmaceutical drug design (based on our analysis of micro-scale intracellular networks) and public health policies for effective interventions during epidemics (based on our study of macro-scale transmission dynamics of epidemic on networks).

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Name	:	**S. Jayakumar**
Enrolment No.	:	LIFE01200804012
Date of Award of degree	:	27.11.14
Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	Molecular Studies on Radiation Response of Human Malignant Cells in Vitro

Abstract

The assessment of tumor radiosensitivity would be particularly useful in optimizing the radiation dose during radiotherapy. This thesis was aimed at understanding the tumor radiosensitivity from the perspective of its prediction and its molecular determinants, so as to personalize the radiotherapy and also to find out the new targets for radiosensitization. For predicting the radiosensitivity, DNA damage as assessed by comet assay and the expression of genes associated with DNA damage response were evaluated for their usefulness in predicting the radiosensitivity of tumor cells. For this purpose, correlation study was performed between the DNA damage assessed by comet assay and clonogenic survival fraction after exposing tumor cells to various doses of gamma radiation (0.5, 1, 2, 4, 6, 8 and 10 Gy) in 7 human tumor cell lines. Among the various parameters analyzed, initial DNA damage measured by neutral comet assay showed significant correlation (r = -0.9) with clonogenic survival of tumor cells. In addition to the acute doses, neutral comet assay showed significant correlation with clonogenic survival fraction after exposure to clinically relevant fractionated doses also (r = -0.93). In order to know the predictive

value of certain genes in assessing radiosensitivity, we have investigated the expression profile of 15 genes involved in crucial radiation response pathways like, DNA damage, repair, apoptosis and redox regulation. Out of 15 genes analyzed, three genes (HSP70, KU80 and RAD51) showed a significant positive correlation with survival fraction. In the study, PC3 and DU145 cells showed differential radiosensitivity as observed by clonogenic survival, apoptosis and neutral comet assays. Therefore, the mechanism of differential radiosensitivity of prostate cancer cell lines PC3 and DU145 was investigated. These cells differed significantly in their radiosensitivity. Both basal and inducible levels of ROS were higher in PC3 cells than that of DU145 cells. DU145 cells showed higher level of basal GSH content and GSH/GSSG ratio than that of PC3 cells. Knock-down experiments and pharmacological intervention studies revealed the involvement of Nrf2-a redox sensitive transcription factor, in differential radio-resistance of these cells, implying that the dysregulation of Nrf2 pathway in tumor cells can lead to radioresistance and in those cells Nrf2 pathway can be a good target for radiosensitization.

Publications

Journal

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Name	:	**Manoj Pralhadrao Remteke**
Enrolment No.	:	LIFE09200604001
Date of Award of degree	:	27.11.14
Constituent Institute	:	Tata Memorial Centre, Mumbai
Title	:	Identification of a Novel ATP Binding Site and Demonstration of ATP Hydrolysis by Mammalian 14-3-3 Isoforms

Abstract

14-3-3 proteins are well known for their ability to bind to phosphorylated residues in proteins and regulate multiple cellular functions. Here for the first time, we show that pure recombinant human 14-3-3C, hydrolyzes ATP with a K_m of 44 pM and a k_{cat} of 0.0087 min^{-1}. Further we show that this ATPase activity is conserved among 14-3-3 y, s and t isoforms and can hydrolyze ATP with similar K_m and k_{ca}, values. In sharp contrast the sigma isoform has no detectable activity. All active 14-3-3 isoforms possess GAR sensor motif. Mutation of a critical Arg (R55A of GAR motif) at the dimer interface in 14-3-3^ reduces ATPase activity. Mutation of D124A in the amphipathic pocket enhances binding affinity and increases k_{ca}, by about 32 fold. This newly identified function may be responsible for some of the physiological roles of 14-3-3 proteins.

Publications

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Name	:	**Joy Mittra**
Enrolment No.	:	ENGG01200704010
Date of Award of degree	:	27.11.14
Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	Structure Property Correlation for Selected High Performance Material

Abstract

Alloy 625, a solid solution strengthened Ni-base alloy, is a preferred candidate for application in high temperature and corrosive environment. Depending upon the temperature and duration of application, a number of ordered phases, such as, $Ni_2(Cr,Mo)$, y" and 5 form in this alloy with attendant change in properties. In this study, growth of these ordered phases and associated changes in coincidence site lattice boundaries due to different isothermal treatments have been correlated with the mechanical properties, including work-hardening behavior. Such correlations have been possible through the microstructural characterizations of isothermally treated and deformed structures using various microscopic techniques and through the analysis of mechanical behavior with support from first-principle based calculations.

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   Materials Science & Engineering A 574 (2013) 86-93.
   DOI: 10.1016/j.msea.2013.03.021
3. CONTRIBUTION OF STACKING FAULT IN LOWERING THE THEORETICAL DENSITY OF NICKEL Joy Mittra, Umesh V. Waghmare, Ashok Arya, Gautam K. Dey
   Computational Materials Science, 81 (2014) 249-252.
4. CORRELATING DISLOCATION-PRECIPITATE INTERACTION WITH WORK-HARDENING BEHAVIOR OF ALLOY 625 Joy Mittra and G. K. Dey (Manuscript communicated)
5. MICROSTRUCTURAL EVOLUTION IN ALLOY 625 DUE TO ISOTHERMAL HOLDING AT HIGH-TEMPERATURES
   Joy Mittra and G. K. Dey (Manuscript ready)
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   Joy Mittra, ASHOK ARYA AND G. K. DEY
   (Manuscript under preparation)

Publication in International Conferences

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   DAE BRNS SYMPOSIUM ON CURRENT TRENDS IN THEORETICAL CHEMISTRY (CTTC-2013), SEPTEMBER 26 - 28,2013, BARC, MUMBAI - 900085.
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Name	:	**Prithwish Tribedy**
Enrolment No.	:	PHYS04201104002
Date of Award of degree	:	27.11.14
Constituent Institute	:	Variable Energy Cyclotron Centre, Kolkata
Title	:	Correlation and Fluctuation of Particle Multiplicity in Hadronic and Heavy Ion Collisions

Abstract

This thesis work includes two major topics: modeling of inclusive multiplicity fluctuations, and measurement of inclusive multiplicity fluctuation in ultra relativistic heavy ion collisions. The goal was to develop an understanding of how observed multiplicity fluctuation arises from different stages of heavy ion collisions. In this work we have developed a new model of initial condition based on the frame work of Color Glass Condensate which naturally describes the inclusive multiplicity distribution in p+p, p+A collisions at RHIC and LHC energies. This model includes various sources of initial state fluctuations and produces eccentricities that are compatible to experimental data of harmonic flow coefficients and can be used as an input to hydrodynamic simulations. We develop method to study inclusive multiplicity fluctuation and correlations in heavy ion collisions. As an experimental investigation of such fluctuations, we present measurement in Au+Au collisions at top RHIC energy on the event-by-event fluctuation and the correlation of the multiplicity of neutral (photons) and charged particles. We study different models and measurement related artifacts on the observables of multiplicity fluctuations. The centrality dependence of the fluctuation in this analysis shows a small but non-zero signal of anti-correlation in the production of charged and neutral particles for mostc entral events. The origin of such fluctuation was investigated using a DCC based model that was implemented using the moment generating function approach. An upper limit of DCC like domain formation in a medium passing through QCD chiral phase transitions in the data sample has been investigated.

Publications

Journal

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   PrithwishTribedyandRaju Venugopalan. Nucl.Phys. A850, 136(2011)[arXiv:1011.1895].
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   A.Bzdak, BjörnSchenke,PrithwishTribedyandRaju Venugopalan.
   Phys. Rev.C87,064906(2013)[arXiv:1304.3403]
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   Nucl.Phys. A904-9052013,409c(2013)[arXiv:1210.5144].
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Name	:	**Ruma Gupta**
Enrolment No.	:	CHEM01201004014
Date of Award of degree	:	27.11.14
Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	Preparation, Characterization and Electrochemical Applications of Modified Electrodes

Abstract

The Thesis entitled "Preparation, Characterization and Electrochemical Applications of Modified Electrodes" by Ms. Ruma Gupta consists of five Chapters. Chapter 1 describes the need of modification of electrode. It includes the introduction to nanomaterials, conducting polymers, carbon nanotubes and their applications. A brief description of fuel cells is given. This Chapter also gives an introduction to the various materials used in nuclear reactors and the significance of analytical characterization of these materials.

Chapter 2 presents the introduction to electroanalytical chemistry, various electroanalytical techniques and the basic fundamental aspects of voltammetric and characterization techniques.

Chapter 3 highlights the synthesis of Palladium nanoparticles on Platinum electrode by employing a potentiostatic pulse method of electrodeposition. The mechanism of electrocrystallization was investigated. The influence of time of deposition on the size and monodispersity of the deposited PdNPs was investigated. The studies revealed that, the size of PdNPs increased with increase in the time of deposition. The PdNPs/Pt was demonstrating enhanced electrocatalytic oxidation of formic acid and methanol for promising performance as catalyst in direct methanol fuel cells and direct formic acid fuel cells.

Chapter 4 describes the use of polyaniline modified platinum electrode (PANI/Pt) to study the influence of ionic speciation in different electrolytic compositions on the performance of the electrocatalysis of PANI/Pt for Fe(III)/Fe(II) redox reaction. PANI-Pt also showed electrocatalytical performance for Pu(IV)/Pu(III) redox reaction because of the cumulative effect of the Donnan interaction between PANI and Pu(IV)-quadra sulphate complex (QSC), specific adsorption of the analyte on the electron transfer centre, higher electron transfer rate constant and catalytic chemical reaction coupled with the electron transfer reaction.

Chapter 5 presents the usefulness of single walled carnon nanotube modified electrode for electrocatalytic performance for Pu, U and Np redox couples. It also showed the fast and simultaneous determination of Pu and U in FBTR fuel samples using SWCNT modified electrodes.

Publications

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1. Influence of ionic speciation on electrocatalysis of fe((III)/fe(II) redox reaction at polyaniline (PANI) coated platinum electrode,
   Saurav Guin, Ruma Chandra and S.K. Aggarwal,
   Electrochimica Acta 55 (2010) 8402.
2. A mechanistic study on the electrocatalysis of the Pu(IV)/Pu(III) redox reaction at a platinum electrode modified with single-walled carbon nanotubes (SWCNTs) and polyaniline (PANI),
   Ruma Gupta, S.K Guin and S.K. Aggarwal,
   RSC Advances 2 (2012) 1810.
3. Electrochemical studies of U(VI)/U(IV) redox reaction in 1 M H2SO4 at single-walled carbon nanotubes (SWCNTs) modified gold (Au) electrode,
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   Ruma Gupta, J.V. Kamat and Suresh K. Aggarwal
   Radiochimica Acta DOI: 10.1515/ract-2014-2273

SYMPOSIUM

1. Influence of Ionic Speciation on Electrocatalysis of Fe(III)/Fe(II) Redox Reaction at Polyaniline (PANI) Coated Platinum Electrode
   Saurav K. Guin, Ruma Chandra, H. S. Sharma and S. K. Aggarwal
   4th ISEAC Triennial International Conference on ElectroAnalytical Chemistry and Allied Topics, edited by S. K. Aggarwal and S. K. Guin, p. 170 (2010).

2. A systematic study on the electrocatalysis mechanism of Fe(III)/Fe(II) redox reaction mediated by polyaniline coated platinum electrode
   Ruma Chandra, Saurav K. Guin and Suresh K. Aggarwal
   4th ISEAC International Discussion Meet on Electrochemistry and its Applications (DM-ISEAC 2011), p 274.
3. Electrocatalytic Mechanism of Pu(IV)/Pu(III) Redox Couple at Single-walled Carbon Nanotubes (SWCNTs) and Polyaniline (PANI) Coated Platinum Electrode,
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   ISEAC International Symposium cum Workshop on Electrochemistry (ISEAC-WS-2011), p 257.
4. Electrochemical studies on utilization of single walled carbon nanotube modified gold electrode for determination of uranium and plutonium
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   64th Annual Meeting of International Society of Electrochemistry (ISE), Sept. 8-13, 2013, Mexico.Poster Number: S-07-036.

Name	:	**Surjya Prakash Ram**
Enrolment No.	:	PHYS03200704011
Date of Award of degree	:	27.11.14
Constituent Institute	:	Raja Rammana Centre for Advanced Technology, Indore
Title	:	Studies on Generation and Manipulation of Laser Cooled Atoms

Abstract

In this work, a double magneto-optical trap (MOT) setup has been developed and made operational for generation of ultracold ^{87}Rb atoms. In the double-MOT setup, transfer of atoms from a vapor chamber MOT (VC-MOT) to an ultra-high vacuum MOT (UHV- MOT) has been extensively investigated during the thesis work. A push beam has been used for transfer of atoms from the VC-MOT to the UHV-MOT in different geometries and configurations to maximize the number of atoms in the UHV-MOT which is useful for evaporative cooling. It has been found that with a low power resonant push beam, the pulsed push beam can result higher number of atoms accumulated in the UHV-MOT than the continuous wave (CW) push beam. The experimental results have been explained on the basis of parameters affecting the atom transfer in both the cases. The investigations during this work also revealed that use of a red-detuned (and higher power) continuous wave push beam of an optimized spot-size results in the maximum number of atoms in the UHV-MOT. The number of atoms transferred to the UHV-MOT is also dependent on the push beam power, its detuning, and capture speed of the UHV-MOT.

Further, the transfer of laser cooled atom cloud from UHV-MOT to a magnetic trap has also been studied during the thesis work. Results showed that the temperature and r.m.s. size of the laser cooled atom cloud in the UHV-MOT and molasses are important parameters that decide the value of optimum magnetic field gradient at which phase-space density in the magnetic trap can be maximized.

To generate the ultracold atomic samples of ^{87}Rb, the evaporative cooling of laser cooled ^{87}Rb atoms in a quadrupole-Ioffe configuration (QUIC) magnetic trap has been performed during the thesis work. After evaporative cooling, a bimodal distribution in the optical density profile of the evaporatively cooled atom cloud was observed which indicated the onset of Bose-Einstein condensation (BEC) in the atom cloud.

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Journal

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3. "Investigation of atom transfer using a red-detuned push beam in a double magneto-optical trap setup", S. P. Ram, S. R. Mishra, S. K. Tiwari and S. C. Mehendale, Rev. Sci. Instrum., 2011, Vol. 82, 126108(1-3).
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6. "Temperature and phase-space density of cold atom cloud in a quadrupole magnetic trap", S. P. Ram, S. R. Mishra, S. K. Tiwari and H. S. Rawat, J. Korean Phys. Soc., 2014 (in Press).

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7. "Optimization of transfer of laser cooled atom cloud to a quadrupole magnetic trap", S. P. Ram, S. K. Tiwari, S. R. Mishra and H. S. Rawat, Proceedings of DAE- BRNS National Laser Symposium (NLS-21), Feb. 6-9, 2013, (BARC, Mumbai).
8. "Push beam spot -size dependence on atom transfer in a double-MOT setup", S. P. Ram, S. K. Tiwari, S. R. Mishra and H. S. Rawat, Proceedings of DAE-BRNS National Laser Symposium (NLS-21), Feb. 6-9, 2013, (BARC, Mumbai).

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Title	:	Vibration Based Robust Condition Monitoring Methods for Rolling Element Bearing - a Signal Processing and Data Based Approach

Abstract

Thesis carries out the research work in the area of condition monitoring of bearings. Vibration signals generated from rolling element bearings are investigated in this thesis to determine the condition of the bearings. The objective is to develop methods for the three phases of condition monitoring: fault detection, fault diagnosis and fault prognosis (degradation).

The existing fault detection methods are noise affected, dependent on sample size, machine and load. Still a simple, efficient and process independent method is required. Fault detection method developed in this thesis tries to solve the above requirements. Two methods of fault detection are discussed. First method uses the signal processing method known as symbolic dynamics to develop a fault index called as Common Signal Index (CSI). Based on the value of CSI, an empirical rule is formed to determine the healthiness of the bearing. Second method uses the Singular Spectrum Analysis (SSA) to compute the singular values of the vibration signal. The ratio of adjacent singular values [singular value ratio (SVR)] is used as a fault detection feature. When the bearing condition changes from healthy to faulty, there is a drastic change in SVR value.

Two approaches for fault diagnosis are developed. The first approach solves the problem of time domain approaches been sensitive to noise and sample size. It is based on the application of SSA and Back Propagation Neural Network (BPNN). Singular values and Energy values obtained using SSA is calculated for healthy and different fault conditions. These values are given as an input to the individual BPNN for the fault classification. In second method, Generalized Teager Kaiser Energy Operator (GTKEO) is used to demodulate the input signal and then followed by spectrum analysis to detect the fault characteristic frequencies. In the fault prognosis study, an index to trend the bearing condition for fault degradation is developed. Performance Index (PI) is obtained using the classifier known as support vector data description and the fault features namely Common Signal Index and Singular Value Ratio which are developed in this thesis.

Thesis contributes mainly the new fault diagnosis method (Generalized Teager Kaiser Energy Operator based), new fault features (Common Signal Index and Singular Value Ratio) and fault degradation index (Performance Index) for the development of an effective prognostic system.

Publications

Journal
a. Published

1. Bubathi Muruganatham, M.A. Sanjith, B. Krishna Kumar and S.A.V. Satya Murty, “Roller element bearing fault diagnosis using singular spectrum Analysis”, Mechanical Systems and Signal Processing, Vol. 35, No. 1-2, pp. 150-166, (February 2013).
2. Bubathi Muruganatham and T. Jayakumar, “Detection of faulty ball bearing using symbolic dynamics”, International journal of Condition Monitoring, Vol. 3, No.1, pp.23-34, (April 2013).
3. Bubathi Muruganatham, S.A.V. Satya Murty, and T. Jayakumar, “Generalized TeagermKaiser Energy operator based bearing fault diagnosis under low SNR and comparison with teager kaiser energy operator”, International Journal of COMADEM, Vol. 16, No.3, pp.3-15, (July 2013).

4. Bubathi Muruganatham, S.A.V. Satya Murty, and T. Jayakumar, "Identification of faulty ball bearings using singular value ratio: case study", International Journal of COMADEM, Vol. 17, No.1, pp.33-42, (January 2014).

b. Communicated

1. Bubathi Muruganatham, S.A.V. Satya Murty, and T. Jayakumar, "Rolling element bearing performance deterioration assessment method using support vector data description" (to International Journal of Prognostics and Health Management).

Conference Proceedings

1. Bubathi Muruganatham, M.A. Sanjith, B. Krishna Kumar, S.A.V. Satya Murty, and P.Swaminathan, "Inner race bearing fault detection using singular spectrum analysis", IEEE International Conference on Communication Control and Computing Technologies ICCCCT '10, October 7-9, Ramanathapuram, India, (2010).
2. Bubathi Muruganatham, C. Sujatha, M.A. Sanjith, T. Jayakumar and B. Krishna Kumar, "Application of singular spectrum analysis for bearing fault diagnosis", National Conference on Condition Monitoring of Engineering Systems & Structures NCCM-2012, June 15-16, Pune, India, (2012).
3. Bubathi Muruganatham, M.A. Sanjith, C. Sujatha and T. Jayakumar, "Symbolic dynamics based bearing fault detection", 2012 IEEE Fifth India International Conference on Power Electronics IICPE 2012, December 6-8, New Delhi, India, (2012).
4. Bubathi Muruganatham, S.A.V. Satya Murty and T. Jayakumar, "Bearing fault diagnosis using generalized teager kaiser energy operator under low SNR", 20t International Congress on Sound and Vibration ICSV20, July 7-11, Bangkok, Thailand, (2013).
5. Bubathi Muruganatham, S.A.V. Satya Murty and T. Jayakumar, "A Method for Rolling Element Bearing Health Degradation Index", National Conference on Condition Monitoring NCCM 2013, October 4-5, Bangalore, India, (2013). (Bubathi Muruganatham)

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Title	:	Synthesis, Characterization and Photoluminesence Spectroscopy of Lanthanide Ion Doped Oxide Materials

Abstract

The work presented in this thesis deals with the synthesis and characterization of a variety of inorganic luminescent materials based on oxides viz. silicate, zirconate, cerate and phosphate. Sm^{3+} and Eu^{3+} behave differently in nanocrystalline ThO_2. Emission spectroscopy shows warm white light emission in $ThO_2:Sm^{3+}$, whereas intense red emission is observed in case of $ThO_2:Eu^{3+}$. Different lanthanide ions viz. Eu, Sm and Dy ions have been used as structural probes to understand their site occupancy in Sr_2SiO_4 and $SrZrO_3$. These ions were found to behave differently in terms of their local site occupancy in these matrices. This aspect has been investigated in detail in the present work. Theoretical modeling and EXAFS studies were carried out to explain such anomaly. TRFS has been extensively used; combined with EXAFS and theoretical calculations to understand the local site symmetry of Eu, Dy and Sm in sol-gel derived Sr_2SiO_4. Based on these studies, it was inferred that Eu^{3+}/ Eu^{2+} occupies both 9- and 10-coordinated Sr^{2+} sites in strontium silicate whereas Dy^{3+} / Sm^{3+} ions occupy only 9-coordinated sites. Nanocrystalline $SrZrO_3$ sample showed defect induced intense violet blue and weak orange red emissions. Based on EPR and theoretical studies, these defects were attributed to presence of shallow and deep defects, respectively. Their corresponding lifetimes were calculated using PL

decay measurements. On doping Sm^{3+} in SZ, an efficient energy transfer takes place and Sm^{3+} ions are localized both at Sr and Zr positions of SZO. In europium doped sample also, europium is distributed between two sites Sr and Zr; HAB (host absorption band) excites mostly Eu at Sr site, CTB (charge transfer band) excites mostly Eu at Zr site, whereas f-f band excites both types of europium equally. In case of Gd/Sm doped SZ samples, Gd prefers Sr^{2+} site and Dy prefers Zr^{4+} site only. Moreover $SrZrO_3:Dy^{3+}$ shows near white light emission: due to presence of blue, yellow and red emissions. Also synthesizing Sr_2CeO_4 is a challenge, because it decomposes peritectically to SrO and $SrCeO_3$ at higher temperatures. Rare earth free blue emitting Sr_2CeO_4 was synthesized which is an efficient blue phosphor. Mechanism for energy transfer and concentration quenching of the PL has been proposed.

Luminescence properties of hosts like ZmP_2O_7 (both undoped and doped) with lanthanide ions have been investigated for the first time with a view to develop new and robust phosphor materials with multifunctional applications. Zinc pyrophosphate is known to undergo structural phase transition at 132^{0}C which was characterized by EPR, HTXRD and DSC. Time resolved emission spectroscopic investigations (TRES suggested that two different types of Eu^{3+} ions (long lived species (1.77 ms) at relatively less symmetric '5-coordinated Zn' sites and short lived species (620 ms) at symmetric '6- coordinated Zn' sites). This was explained with the help of Judd-Ofelt (J-O) calculations, which revealed that the radiative life time of the Eu^{3+} species present in symmetric environment was higher than that of the species present in asymmetric environment. It was observed that the presence of a strong non-radiative component at the symmetric site brings down the overall lifetime value.

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2. "Understanding the local environment of Sm3+ in doped SrZrO3 and energy transfer mechanism using time resolved luminescence: A combined theoretical and experimental approach", Santosh K. Gupta, P. Ghosh, N. Pathak, A. Arya, V. Natarajan, RSC Advances,4 (2014) 29202
3. "A Novel near white light emitting nanocrystalline Zn2P2O7: Sm3+ derived usingcitrate precursor route: Photoluminescence spectroscopy", ", Santosh K. Gupta, N. Pathak, M. Sahu, V. Natarajan , Advanced powder Technology , 25 (2014) 1388-1393
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14. "Site specific luminescence of Eu3+ in gel combustion derived strontium zirconate perovskite nanophosphors", S.K. Gupta, M. Mohapatra, V. Natarajan and S.V.Godbole, Journal of Materials Science, 47 (2012) 3504-3515
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16. "Probing local site occupancy of various lanthanide ions (Eu3+,Dy3+ and Sm3+) in a-Sr2SiO4 host: TRFS, EXAFS and Theoretical calculations", Santosh K Gupta, Sandeep Nigam, A. Yadav, M. Mohapatra, S.N. Jha, C. Majumader, D. Bhattacharya, V. Natarajan, Inorganic Chemistry (Communicated)

National and International Symposia:

1. Structural phase transition in zincpyrophasphate: EPR and HTXRD investigations, Santosh K. Gupta, R.M. Kadam, V. Natarajan and S. V. Godbole, International symposium on materials chemistry, ISMC-2012, Mumbai, Dec-2012
2. Synthesis and Photoluminescence properties of Eu3+:Sr2SiO4, , Santosh KumarGupta, M. Mohapatra, V. Natarajan, and S.V.Godbole, International conference on luminescence and its application (ICLA-2012), Hyderabad, Feb-2012(Best poster award)
3. Europium doped zinc pyrophosphate: Photo and Thermoluminescence, , Santosh K. Gupta, B. Sanyal (FTD), V. Natarajan, and S.V. Godbole, National conference on luminescence and its application (NCLA-2012), Bangalore, Jan-2013 Oxidation State Of Manganese in Zinc Pyrophosphate: Probed By Luminescence An EPR Studies, Santosh K. Gupta, R.M. Kadam, V. Natarajan and S. V. Godbole, Solid state physics symposium, SSPS-2013, Patiala, Dec-2013
4. Optical and magnetic properties of nanocrystalline SrZrO3, Santosh K. Gupta, P. Ghosh, N. Pathak, R.M. Kadam, A. Arya, V. Natarajan, ICONSAT-2014, INST, Chandigarh, march-2014
5. Local site symmetry of Sm3+ in α'-Sr2SiO4: Probed by emission and fluorescenc lifetime spectroscopy, Santosh K. Gupta, N. Pathak, S.K. Thulasidas, V. Natarajan, ICL-2014, Wroclaw, Poland, July 2014

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Title	:	Understanding Creep Deformation Behavior of 316LN Stainless Steel and its Weld Joint Using Impression Creep Technique

Abstract

Impression creep technique is an innovative material non-invasive, small specimen testing technique that can be used for evaluating creep properties of materials. The technique enables probing small volume of material in relatively short test time. Hence, impression creep technique is attractive for rapid screening of creep properties of several laboratory heats for optimizing chemical compositions in development of new alloys and is uniquely suitable for determining creep deformation characteristics of narrow microstructural zones of weld joints.

The thesis discusses the development and establishment of the impression creep testing system at IGCAR. To validate the technique, systematic studies have been carried out on the creep deformation behavior of 316LN SS and its weld joint using this technique. Impression creep tests were carried out on 316LN SS under different stress levels in the range 472-760 MPa, at various temperatures in the range 898-973 K, using specimens of dimension 20 mm x 20 mm x 10 mm, under vacuum of 10^{-6} mbar. Cylindrical indenters with flat-end, made of tungsten carbide, were used and the diameter of the indenter was 1 mm. Impression creep curves exhibited a primary creep stage and a secondary creep stage. Equivalence between the punching stress and steady state impression velocity with uniaxial stress and steady state creep rate respectively has been established. Stress dependence of creep deformation in 316LN SS was investigated. The Norton power law relationship was found to be obeyed between steady state impression velocity and punching stress. The temperature dependence of creep deformation in 316LN SS was investigated and Arrhenius-type rate equation was found to be followed between steady state impression velocity and temperature. The apparent activation energy determined for creep deformation was found to be in close agreement with the apparent activation energy obtained from the uniaxial creep tests.

In order to optimize nitrogen content in 316LN SS the effect of nitrogen on creep properties of 316LN SS has been evaluated by employing impression creep technique as a faster and non-invasive method. Impression creep tests were conducted at 923 K on different heats of 316LN SS containing 0.07, 0.11, 0.14 and 0.22 wt. % nitrogen, under different punching stress levels. The steady state impression velocity was found to decrease with increasing nitrogen content at all the punching stress levels. Impression creep testing technique was found to be sensitive to capture the small variation in creep rate due to the small change in chemical composition of the alloys.

Impression creep technique was employed to characterize creep behavior of different microstructural zones of a high nitrogen grade of 316LN SS weld joint. The tests were carried out at 923 K on three distinct microstructural zones, namely, the weld metal, the heat-affected zone and the base metal of a 316LN SS weld joint, at the same stress levels. The weld metal, the base metal and the heat-affected zone exhibited different creep rates. The difference in creep behavior of each zone was correlated with the difference in microstructure and morphology of different zones of the weld joint. Equivalent steady state creep rates for the base metal and weld metal obtained from impression creep tests were in good agreement with the steady state creep rates for the base metals and the weld metals determined from conventional uniaxial creep tests.

Extensive studies on the size and shape of the developed plastic zone, the evolution of stress under the punch during elastic, plastic and creep process, onset of plastic deformation, the dynamics of the material flow in response to the indentation and the mechanism of material pile-

up on the specimen surface during impression creep test have been carried out using experimental and finite element simulation studies.

Publications

I. Peer Reviewed International Journals

1. Naveena, V. D. Vijayanand, V. Ganesan, K. Laha and M. D. Mathew, "Evaluation of The Effect of Nitrogen on Creep Properties of 316LN Stainless Steel from Impression Creep Tests", Materials Science and Engineering A 552 (2012) 112-118.
2. M.D. Mathew, Naveena, and D. Vijayanand, "Impression Creep Behavior of 316LN Stainless Steel", Journal of Materials Engineering and Performance, 22(2) (2013) 492-497.
3. Naveena, V.D. Vijayanand, V. Ganesan, K. Laha and M.D. Mathew, "Application of Impression Creep Technique for Development of Creep Resistant Austenitic Stainless Steel", Procedia Engineering, 55 (2013) 585-590.
4. Naveena, V.D. Vijayanand, K. Laha and M.D. Mathew, "Evaluation of Creep Deformation Behavior of Different Microstuctural Zones of 316LN SS Weld Joint using Impression Creep Testing Technique", Materials Science and Technology, 30 (2014) 1223-1228.
5. Naveena, P. Parameswaran, K. Laha and M.D. Mathew, "Study on creep deformation mechanism of 316LN stainless steel from impression creep tests", Materials at High Temperatures, 31(2) (2014) 180-184.
6. Naveena, J. Ganesh Kumar and M.D. Mathew, "Finite element analysis of plastic deformation during impression creep", Journal of Materials Engineering and Performance, (2014) in print.
7. Naveena, Vani Shankar, P. Parameswaran and M.D. Mathew, "Impression creep deformation behavior of 316LN stainless steel", Materials at High Temperatures, (under review).
8. M.D. Mathew, Naveena and J. Ganesh Kumar, "Evaluation of tensile, creep and fracture toughness of materials using innovative small specimen testing methods" Materials at High Temperatures (under review)

II. Conference Proceedings

1. Naveena and M.D. Mathew, "Effect of Nitrogen on Creep Deformation Behavior of Type 316 LN Stainless Steel: Studies Using Impression Creep Technique", Proc. 12th International Conference on Creep and Fracture of Engineering Materials and Structures (CREEP 2012), Kyoto, Japan, May 25-31, 2012.
2. Naveena and M.D. Mathew, "Equivalence Between Impression Creep and Uniaxial Creep in 316LN SS", Proc. 49th National Metallurgists' Day (NMD) and the 65th Annual Technical Meeting (ATM) of the Indian Institute of Metals (IIM), Hyderabad, India, November 13-16, 2011.
3. Naveena, V. D. Vijayanand, K. Laha and M. D. Mathew, "Impression Creep: An Innovative Testing Technique for Characterizing Creep Behavior of Weldments", Proc. the 5th National Symposium for Materials Research Scholars (MR-13), IIT Bombay, India, May 8-10, 2013.
4. M.D. Mathew and Naveena "Understanding Creep Deformation Behavior of 316LN Stainless Steel from Impression Creep Tests, Proc. 16th International Conference on Strength of Materials, ICSMA-16, Bangalore, India, August 19-24, 2012.
5. M.D. Mathew, K. Laha, J. Ganesh Kumar and Naveena, "Innovative Mechanical Testing Techniques for Evaluation of Creep Properties of Materials", Proc. International Conference & Exhibition on Pressure Vessels and Piping - OPE-2013, Mamallapuram, Tamil Nadu, India, February 13-16, 2013.

III. Report

1. Evaluation of Creep Deformation Behavior of 316LN Stainless Steel and Its Weld Joint using Impression Creep Technique, IGC Newsletter, Vol. 101 (2014) 22-26.

IV. Awards and Recognitions

1. "Young Researcher's Award" from The Indian Institute of Metals, Kalpakkam Chapter, for the year 2012, for the paper "Evaluation of The Effect of Nitrogen on Creep Properties of 316LN Stainless Steel from Impression Creep Tests" by Naveena, V. D. Vijayanand, V. Ganesan, K. Laha and M. D. Mathew, Materials Science and Engineering A 552 (2012) 112– 118.

2. "Best Poster Paper award" in the 6th International Conference on Creep, Fatigue and Creep-Fatigue Interaction held during January 22-25, 2012 at Mamallapuram, Tamil Nadu, India, for the paper "Application of Impression Creep Technique for Development of Creep Resistant Austenitic Stainless Steel" by Naveena, V. D. Vijayanand, V. Ganesan, K. Laha and M. D. Mathew.
3. Awarded "International Travel Support Fellowship" from Science and Engineering Research Board, Department of Science and Technology (DST), Govt. of India, to attend and present the research paper in the 12th International Conference on Creep and Fracture of Engineering Materials and Structures (CREEP 2012) held during May 25-31, 2012, in Kyoto, Japan.

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Title	:	Development of Materials and Coating Technology for Pyrochemical Reprocessing Plant Applications

Abstract

Metallic fuelled Fast Breeder Reactors (FBR) with co-located pyrochemical reprocessing plants have been proposed as the best option to increase the breeding gain, reduce the doubling time of the fuel and reprocess short cooled and high burnup fuel. The major part in implementation of the pyrochemical reprocessing technology involves identification, development, testing and qualification of reliable corrosion resistant materials/coatings for service in corrosive molten LiCl–KCl eutectic salt operating at 500 to 600°C for salt purification and electrorefining operations. Selection of reliable materials and coatings for fabrication of equipment in pyrochemical reprocessing is of major importance as these processes are carried out remotely under intense radiation, and maintenance & repair are not feasible. The study evaluated the corrosion behaviour of candidate materials in molten LiCl–KCl eutectic salt under Cl_2, air and ultra high purity argon environments. Weight loss results indicated that the corrosion resistance of the materials increased in the following order 2.25Cr-1Mo < 9Cr-1 Mo < Inconel 600 ~ Inconel 690 ~ Inconel 625 < YSZ coating < Pyrolytic graphite in molten salt under ultra high purity argon environment. Inconel 600 and Inconel 690 offered better corrosion resistance in molten LiCl–KCl salt under air environment compared to Inconel 625, while Inconel 690 offered better corrosion resistance in molten LiCl–KCl salt under chlorine environment. Characterisation of corroded surfaces and scales by XRD, SEM and EDX aided in identifying the morphology, composition and phases of corrosion products and understand the degradation behaviour. The study revealed intergranular corrosion, corrosion along twin boundaries and preferential dissolution of precipitates within the grain, for Inconel 600 and Inconel 625 exposed to molten salt under Cl_2 bubbling while welds revealed interdendritic dissolution. The mechanism of corrosion of Cr-Mo steels, 316L SS & Ni base alloys in molten salt under air and argon atmosphere was found to be due to selective dissolution of Cr with eventual formation of voids and formation of chromium rich compound at the surface and subsequent spallation. Since metallic materials exhibit poor performance in molten salt environment at high temperatures, corrosion protection coatings such as plasma sprayed partially stabilized zirconia (PSZ) has been proposed. PSZ coating tested in molten LiCl–KCl eutectic salt exhibited excellent corrosion resistance. In order to improve the durability of the coatings optimization of plasma spray process parameters through co-injection of bond coat and ceramic coat powders using single torch has been carried out. Graded region without reaction of bond coat with PSZ and oxidation of bond coat was achieved as indicated

from the back scatter SEM micrograph, EDX line profile and X-ray elemental mapping. Graded coating exhibited marginally higher adhesion strength compared to duplex coating. Post surface treatment of PSZ coatings such as laser remelting has also been attempted to densify the surfaces in order to improve the corrosion resistance. Laser remelting of PSZ coatings resulted in dense, smooth and hard surface with beneficial non-transformable t' phase.

Publications

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1. A. Ravi Shankar and U. Kamachi Mudali, Corrosion of 316L Stainless Steel in Molten LiCl–KCl Salt, Materials and Corrosion, 2008, 59 (11) pp 878- 882.
2. A. Ravi Shankar and U. Kamachi Mudali, Laser Surface Modification of Plasma Sprayed Yttria Stabilized Zirconia Coatings on Type 316L Stainless Steel, Surface Engineering, 2009, 25 (3) pp 241-248.
3. A. Ravi Shankar, S. Mathiya, K. Thyagarajan and U. Kamachi Mudali, Corrosion and Microstructure Correlation on Materials in Molten LiCl–KCl Medium, Metallurgical and Materials Transactions-A, 2010, 47 (7) pp 1815-1825.
4. A. Ravi Shankar, A. Kanagasundar and U. Kamachi Mudali, Corrosion of Nickel Containing Alloys in Molten LiCl–KCl Medium, Corrosion, 2013, 69 (1) pp 48-57.
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2. A. Ravi Shankar and U. Kamachi Mudali, Laser Consolidation of Plasma Sprayed Yttria Zirconia Coatings on Type 316L Stainless Steels, Poster Presentation for The Indian Institute of Metals, NMD-ATM 2007, 61th Annual Technical Meeting, 13-16 Nov, 2007, Mumbai.
3. A. Ravi Shankar, S. Mathiya and U. Kamachi Mudali, Corrosion of Materials in Molten LiCl–KCl Medium, Proceedings for Fourteenth National Congress on Corrosion Control, September 18-20, 2008, Hyderabad.
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5. U. Kamachi Mudali, A. Ravi Shankar and S. Ningshen, “Plasma Sprayed Thermal Barrier Coatings for Molten Chloride Environment”, Proc. SMT-25, Sweden, 20-22 Jun 2011.

3. REPORTS

1. U. Kamachi Mudali, A. Ravi Shankar, C. Mallika, K. Thyagarajan, S. Ningshen, B.P. Reddy and K. Nagarajan, “Materials and Coating Technologies for Pyrochemical Reprocessing of Spent Metallic Fuel from Fast Breeder Reactors” Technical Report submitted to Director IGCAR, September 2011.

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Title	:	Identification of Protein Interaction Networks of Gankyrin in Cancer

Abstract

Protein-protein interactions create highly dynamic, spatio- temporal functional networks. Many oncogenes and tumor suppressors act as hubs in the functional network and are capable of rewiring the network leading to an altered phenotype. Since rewired networks are unique to cancer cells, these specific interaction sites become very important drug targets. Therefore, we aim to identify the physiological relevant direct interacting partners of gankyrin which is known to be over expressed in several epithelial cancers. Based on the principles of sequence conservation and the role of key residues in dictating the binding affinity at protein interfaces, we predicted novel putative interacting partners of gankyrin. In order to map the gankyrin interaction network, we capitalized on available crystal structure of a mouse gankyrin-human S6ATPase complex. We recognised a potential hot spot site made of tetrapeptide sequence 'EEVD' at the interface. Hence, we hypothesized that gankyrin might interact with proteins having EEVD/EEXD in the well exposed region. Interactions of gankyrin with eight proteins NCK.2, G-rich RNA sequence binding factor 1 (GRSFI), Chloride intracellular channel protein 1 (CLIO), Eukaryotic initiation factor 4A-III (EIF4A3), dimethylarginine dimethylaminohydrolase 1 (DDAH1) and mitogen- activated protein kinase I (MAP2K1), Hsp70, Hsp90 were validated inside the cellular milieu. Interacting partners form the complex with gankyrin which is stabilized by interactions through linear short stretch of four amino acids. Three of the interactions (CLIO, MAP2K1. DDAHI) occur only when gankyrin is over expressed or in cancerous cell lines where gankyrin is known to play a vital role. Mutagenesis experiments confirm that these interactions involve the predicted residues which form the hotspot sites at the shared interface and could be a potential drug target. In the Short Linear Sequence Motif EEVD we found that Val at the gankyrin-S6ATPase interface is probably less important for the interaction. Hence, we expanded our prediction to EEXD containing proteins- Calreticulin (EEMD). Calreticulin is an endoplasmic reticulum residing protein and found to be over expressed in hepatocellular carcinoma tissues. Gankyrin interacts with calrecticulin through E, F. and D residues of EEMD sequence and the interaction was specific to gankyrin over expressing cells. We further went ahead with understanding the functional significance of the gankyrin-CLICI interaction. Knockdown and rescue experiments proved that gankyrin interaction with CLICI through E, E and D show enhanced migratory properties in MDA-
MB-231 cells.

Publications

Journal

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Title	:	Synthesis and Characterization of Nanophosphor for Radiation Detection and Dosimetry

Abstract

Lanthanum Fluoride doped with Cerium has received attention in the field of luminescence as well as radiation detection for its absorption of higher energy radiation, high light emission, and silent host lattice with low phonon energies preserving the activator site and possessing fast decay time. Nano size will add strength towards more light intensity. Nano sized LaF_3:Ce was synthesized in four different routes. Initially in order to achieve nano size, surface modification of LaF_3:Ce was carried out using Oleic acid (OA) and the combination of Polyethyelne glycol (PEG) and OA. Nano size was successfully achieved by applying surfactants but at the cost of light output. In order to achieve both nano size and higher light output, LaF_3:Ce was synthesized in acidic environment without any coating. Acidic environment yielded nano particles with very narrow size distribution. Various uncoated samples of LaF_3:Ce were synthesized with upto 0.45 mol. A red shift in the PL spectra was observed at higher Ce concentration. Uncoated particles showed five distinct, clearly resolved absorption peaks at wavelengths 198, 205, 218, 234 and 247 nm. For the first time LaF_3:Ce had nano size with very narrow distribution possessing very high light output. The PL output (300 – 325 nm) of Cerium was significantly converted to a visible light (543 nm) by codoping with Terbium through Energy transfer from Cerium to Terbium. Life time of the PL emission of nano sized LaF_3:Ce was found to be 25 ns.

TiO_2 has been successfully coated upon the nano sized $La_{0.40}F_3:Ce_{0.45}^{3+},Tb_{0.15}^{3+}$, $La_{0.55}F_3:Ce_{0.45}^{3+}$ and $La_{0.85}F_3:Tb_{0.15}^{3+}$ matrices to obtain a core-shell structure. The core-shell structure formation was confirmed with TEM images and FTIR spectra. The effect of TiO_2 coating thickness on PL intensity was studied. About 1.76 times increase in the light output (543 nm) was observed at a coating thickness of 4-6 nm. Scintillation under X-ray excitation was observed from the uncoated and coated $La_{0.40}F_3:Ce_{0.45}^{3+},Tb_{0.15}^{3+}$ matrices.

The effect of non-stoichiometry of LaF_3 on the PL behavior was studied by varying the molar ratios of $LaCl_3$ and NH_4F. Changes in the particle size as well as the PL spectra and intensity were observed due to nonstoichiomety. This indicates towards a possibility of introducing tunability by changing the stoichiometry.

The radiation induced degradation of nano sized $LaF_3:Ce^{3+}$ which in turn affects their performance as a radiation detector. As the proposed primary application of this material is radiation detection, it requires radiation stability with respect to the PL behavior. Reduction in UV-Vis absorption and PL intensity were observed to follow a similar decreasing trend in both coated and uncoated nanocrystals subsequent to γ- radiation. TL measurements were carried out on $LaF_3:Ce^{3+}$nanocrystals, after annealing. TL peak appears at 409° K (136ºC), indicating dosimetriclly a useful peak. TL decay kinetics follows a second order indicating Gaussian nature of the traps formed to trap more ions, which recombine to give more light. The trap depth was calculated for the main peak at 409° K using Chen's equation is 0.57 eV. The results are highly promising towards using these crystals for radiation dosimetry.

The main objective of the work was achieved by preparing radiation sensitive transparent polymer nanocomposite (PNC) material. Polyacrylamide as well as Polymethylmethacrylate (PMMA). PNC materials were prepared using the coated as well as uncoated synthesized nanoparticles and their PL properties measurements were carried out. The microscopical and FESEM micrograph observations indicated an uniform particle distribution in the PNC matrix. The TiO_2 coated $La_{0.4}F_3:Ce_{0.45},Tb_{0.15}$ embedded in PMMA shows a better performance in terms of

particle distribution as well as light output. For the first time, scintillation of uncoated and TiO_2 coated $La_{0.4}F_3:Ce_{0.45},Tb_{0.15}$ PMMA composite under X-ray excitation was observed.

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1. T.K. Srinivasan, B. Venkatraman, D.Ponraju and A.K.Arora, "Photo luminescent characteristics of oleic acid coated LaF_3:Ce embedded in Polyarylamide", World Journal of Nano Science and Engineering. 2 (2012) 201.
2. T.K. Srinivasan, B.S. Panigrahi, A.K. Arora, B. Venkatraman and D.Ponraju, "Gamma irradiation effect on Photoluminescence from functionalized LaF_3:Ce nanoparticles", Radiation Physics and Chemistry 99 (2014) 92-96
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1. T.K. Srinivasan, D. Ponraju, B. Venkatraman and A.K. Arora, "Effect of gamma irradiation on Oleic acid coated LaF_3: Ce on nano phosphor" National Symposium on Radiation Physics and Nanomaterials (NSRPN), p 187, (2011) at Patiala, Punjab, INDIA.
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Title	:	Modelling and Simulation of Hybrid Membrane Separation System

Abstract

Membrane processes are continuously gaining importance owing to several advantages including eco-friendliness, modularity, low chemical intervention, low maintenance and uni-phase operation. One step pressure driven membrane processes such as reverse osmosis, nano-filtration and ultra-filtration are the work horses in the water treatment industry today meeting the objective of providing purified water but they do not lead to absolute separation. They have

still some environmental challenges to overcome with regard to the disposal reject streams. In this context, it is felt appropriate to use hybrid membrane processes which combine two membrane processes with same or different characteristics operating in tandem. Accordingly it was decided to take up the study of hybrid membrane separations in detail which forms the subject matter of the doctoral work. The various studies and developments were presented in four chapters.

The introductory chapter describes various membrane based separation processes with emphasis on pressure driven processes. The different mechanisms of the processes proposed for the pressure driven processes such as sieve mechanism, wetted surface mechanism, solution-diffusion mechanism and preferential sorption capillary flow mechanism are reviewed in detail. The various mathematical models which describe the transport of solute through the membranes were then presented. The concept of irreversible thermodynamics model has been analysed in detail particularly based on Kedem-Katchalsky and Spiegler-Kedem approaches. Even though the whole range of pore-sizes are covered from molecular size in RO to about a few microns in MF, absolute separation is hardly possible particularly from homogeneous systems. Highlighting the necessity to look for a combination of processes to achieve near absolute separations, two challenging industrial problems particularly relevant to nuclear industry namely 'Removal or separation of trace contaminant from effluent stream' and 'Recovery of water from near saturated sparingly soluble effluent stream for reuse' have been chosen as the subject matter of the thesis with specific objectives on experimental studies to generate separation characteristics and thereafter modeling and simulation of the same based on the membrane characteristics, solute characteristics and hydrodynamics.

The second chapter describes the work carried out with respect to the 'Removal or separation of trace contaminant from effluent stream'. Starting from the literature model based on irreversible thermodynamic approach, the modifications carried out step by step are described. The base model treats membrane as a black box and describes the water flux and solute flux through two coefficients $\acute{\sigma}$ (reflection coefficient), $\acute{\omega}$ (solute permeability) respectively. The experimental studies were carried out using complexation-ultrafiltration. The complexation-ultrafiltration operates on the principle of increasing the size of the species to be removed followed by ultrafiltration. In the studies the separation of copper was investigated with polyethyleneimine (PEI) as a complexing ligand, using UF with different MWCO (6,20 and 100KD). The detailed studies indicated that the separation depends on pore size distribution of the membranes, molecular weight distribution of complexing ligand and stability constant of Cu-PEI complex (K_d) of the metal ligand complex. The model was developed incorporating the discretised pore size distribution of the membrane and molecular weight distribution of ligand and stability constant into the basic Kedem Katchalsky model and validated based on the experimental studies with copper. The model equations were applied to predict the removal of cobalt and iron as single contaminants and later fractionation of cobalt-iron mixed solute. The combination two UF membranes with different MWCOs were optimized to provide higher separation of Co and iron. The experimental results were found to be in good agreement with the model predictions.

The third chapter deals with the experimental studies on the use of hybrid membrane system to recover water and value from mining effluent circumventing the scaling of $CaSO_4$ and the development of a simulation model. Application of NF prior to RO is a critical step in which most bivalent load was eliminated by high flux NF keeping RO at minimum scale threat. Experimental studies were conducted to locate the critical point of flux decline owing to calcium sulphate scale formation in NF. Further it was established that the critical point was only dependent on feed concentration and recovery and is independent of flow rates. From the experimental data, empirical correlation of resistance as a function of feed flow, product flow, operating pressure and reject concentration were developed using least square regression method. Based on the correlation and experimental observations, a simulation model was developed to optimise the operating parameters namely the feed flow rate and operating pressure for a given feed composition. A mathematical model of reverse osmosis for optimizing, the operating pressure,

required product quality and quantity have been incorporated. Studies pertaining to optimising the hydrodynamic parameters by thermodynamic exergy calculation and reject management were also carried out. Reject management studies with reference to NF concentrates using lime column has been carried out to demonstrate the approach to zero liquid discharge.

The last chapter provides the summary and conclusions indicating that it was possible to remove trace contaminants particularly heavy metals by complexation UF. With judicial combination of two UF systems it was demonstrated that the mixed systems also can be fractionated. The model developed incorporating the pore-size distribution of the membrane and molecular weight distribution of the complexing ligand along with the stability constant of the metal – ligand complex could reasonably predict the behaviour not only for single component but also for mixed solute systems. In the case of saturated calcium sulphate effluent stream it was indicated that a NF-RO system combined with lime column could lead to near zero liquid discharge.

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Title	:	Theoretical Developments and Studies in the Reactor Physics of Accelerator Driven System

Abstract

The thesis presents theoretical work and development of computer codes aimed towards studying Accelerator Driven Sub-critical Systems (ADS) and in particular towards designing and planning experiments for measurement of the sub-criticality in ADS by deterministic and stochastic methods. In the internationally proposed experiments like pulsed neutron or noise based experiments, the neutron flux distribution is a mixture of several alpha modes which decay at different characteristic rates; the slowest one being of particular interest as it can be related to the sub critical reactivity. For avoiding contamination of detector response due to higher modes, knowledge of the location of the zeros of the higher alpha modes is very useful. This needs an evaluation of the higher alpha modes. New numerical schemes for the evaluation of higher alpha modes have been worked out. A new scheme is developed to extend the method for super-critical systems. In addition to alpha mode evaluation, a three dimensional space time kinetics code to predict reactor behaviour during transients has been developed. The code can also perform stochastic kinetics analysis for simulating noise experiments and can calculate Rossi alpha and Feynman alpha through the use of time dependent adjoint functions. For simulating noise experiments in ADS, a transport theory equivalent analogue Monte Carlo code has also

been developed. The code has been validated by comparing with criticality benchmarks and with results of a simulator code based on diffusion Monte Carlo, as well as with Feynman alpha and Rossi alpha calculations based on solutions of the forward and adjoint equations.

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Name	:	**Arijit Sengupta**
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Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	Studies on the Extraction/Complexation of Actinide and Fission Product Elements Using Selective Ligands in Room Temperature Ionic Liquids

Abstract

The Thesis entitled "Studies on the extraction/ complexation of actinide and fission product elements using selective ligands in room temperature ionic liquids" by Mr. Arijit Sengupta consists of six Chapters. The introductory Chapter gives an overview of the nuclear fuel cycle, the impact of various types of nuclear wastes on the Environment. Actinide chemistry including electronic configuration, ionic species, variable valency, disproportionation etc was discussed. A brief introduction of RTILs and its application in nuclear fuel cycle are discussed. This Chapter also lists the motivations for the present study.

Chapter 2 deals mainly with instrumentation, materials and methods. The brief description of the instruments, optimization of instrumental and experimental parameters, working principles of different techniques and synthesis / source of different ligands and RTILs are discussed.
In Chapter 3, extraction of actinides by solvents containing multiple-DGA-functionalized ligands in different RTILs was studied from acidic feed solution and the results were compared with TODGA. The unusually high extraction of Am^{3+} can be attributed to the unique cation-exchange mechanism in the RTIL medium with 1 : 1 complexes having no inner sphere water molecules, while the high viscosity of the RTILs is responsible for the slower extraction kinetics. EDTA/ DTPA in guanidine carbonate were successfully used for quantitative stripping of Am^{3+}.

Chapter 4 presented the effects of structural modification in ligand as well as in both cationic and anionic parts of RTILs on the extraction properties of actinides. It also included the studies on extraction mechanism, kinetics, nature of species involved in separation (e.g. inner sphere or

outer sphere complex) and the thermodynamics associated with the extraction. Time resolved fluorescence spectroscopy, theoretical computation and cyclic voltammetry were also employed for better understanding of the complexation in RTIL medium.

Chapter 5 reported the studies on the extraction and complexation properties of diglycolamide functionalized RTIL with different oxidation states of actinides and its comparison with CMPO functionalized RTIL

Chapter 6 included the studies on the recovery of ^{90}Sr using substituted crown ethers in RTILs. Finally all the RTIL based solvent systems were applied for actinide partitioning from simulated radioactive waste solution.

The thesis ended with the summary and conclusion chapter with future prospective.

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13. Spectroscopic investigation of Eu^{3+} - complexes with ligands containing multiple diglycolamide pendant arms in a room temperature ionic liquid Arijit Sengupta, Prasanta K. Mohapatra, Mudassir Iqbal, Jurriaan Huskens, Willem Verboom, J of Luminescence, 154 (2014)392 - 401.
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2. Extraction and radiolytic degradation studies using a novel actinide selective solvent system containing a tripodal diglycolamide in room temperature ionic liquids. A. Sengupta, M. Iqbal, W. Verboom, and P.K. Mohapatra, SESTEC (2012).
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10. Spectroscopic investigation of Eu^{3+} - complexes with ligands containing multiple diglycolamide pendent arms in room temperature ionic liquid. Arijit Sengupta, P.K.Mohapatra, Mudassir Iqbal, Jurrian Huskens, Willem Verboom, SESTEC (2014).
11. Studies on the complexation of UO_2^{2+} with DGA-TSIL. Arijit Sengupta, M.S.Murali, P.K.Mohapatra, Mudassir Iqbal, Jurrian Huskens, Willem Verboom, SESTEC (2014).
12. Study the complexation of Np(IV) with task specific ionic liquids by cyclic voltammetry. Arijit Sengupta, M.S.Murali, P.K.Mohapatra, Mudassir Iqbal, Jurrian Huskens, Willem Verboom, SESTEC (2014).
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15. Separation of Lanthanides and actinides from Simulated High Level Waste using diglycolamide-functionalized calix[4]arene Arijit Sengupta, P.K.Mohapatra, Mudassir Iqbal, Jurrian Huskens, Willem Verboom, NAC -5 (2014).

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Title	:	Design and Development of High Current Radio-Frequency Quadrupole Accelerator

Abstract

Radiofrequency quadrupole (RFQ) accelerators are extensively used as injectors in the high-current Linacs because of their remarkable capability of simultaneously focusing, bunching and accelerating the low-energy ion beams with high transmission and minimum emittance growth. However, in all the RF accelerators the beam must be longitudinally bunched so that all particles are accelerated. Before the invention of RFQ, the bunching of beam was accomplished prior to injection into the Linac using one or more RF buching cavities. In buncher cavities RF electric fields are applied to the DC input beam to produce a velocity modulation in which early particles are decelerated and late particles are accelerated. After a suitable drift space, the beam becomes bunched, ready for injection into the Linac. The bunching is usually not very efficient (ie, Transmission < 40 %), especially for high-current beams because of the higher space-charge forces at low energies. In high-intensity beams, the bunching process causes an increase in the beam density, which increases the space-charge forces and often results in transverse emittance growth. However, the RFQ eliminates these problems by employing the adiabatic bunching process, which increases the capture efficiency of the RFQ to nearly 100 %. Because of their high capture efficiency at low energies, the RFQs suite well as a first unit of high current RF linear accelerators in applications, such as production of Radio-active ion beams, Accelerator Driven Systems (ADS) for effective utilization of thorium resources and Spallation Neutron Source (SNS). In view of the importance of RFQ accelerators for high current machines, the R&D activities for the design and development of 400 keV deuteron and 3 MeV Proton RFQs (four-vane type), were initiated at BARC, Mumbai. These RFQs are planned to operate in CW mode.

The deuteron RFQ operates at a resonant frequency of 350 MHz, and needs an intervane voltage of 44 kV to accelerate the beam to final energy of 400 keV over a vane length of 1.03 m. The RF power needed to generate the vane voltage of 44 kV was ~ 55.5 kW. The effects of mechanical errors on the field distribution are studied using a perturbative analysis based on 5 wire transmission line theory. Based on this theory a computer program has been written for tuning this RFQ. The RFQ made of OFHC copper have been machined and vacuum brazed indigenously at BATL, Trivandrum. Initially the low power test (ie., Q factor and field tuning) was done. After the successful completion of low power tests, the high power conditioning (pulsed mode) and beam acceleration experiments were done on this RFQ. The output energy of the deuteron beam was measured with a bending magnet and transmission of 94 % was obtained and the results are in good agreement with the simulations.

The proton RFQ operates at a resonant frequency of 352.21 MHz, and needs an inter-vane voltage of 68 kV to accelerate the beam to final energy of 3 MeV over a length of 4 m. The main criteria while designing these RFQs were, (a) maximize the beam transmission (b) Minimize the emittance growth (c) Minimize the length (d) Minimize the peak surface field in order to reduce the sparking.

In this thesis, the design aspects of both 400 keV and 3 MeV RFQs, RF and beam characterization of the 400 keV RFQ are discussed. The parameters of the 3 MeV RFQ was finalized and its fabrication is in progress.

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Abstract

Charmonium production had been identified as one of the most promising diagnostic probes to indicate the occurrence of the de-confinement phase transition in relativistic nuclear collisions. The present thesis deals with the production of charmonia and the feasibility of their detection via di-muon channel, at energies available from the upcoming FAIR accelerator facility. The work is broadly divided into two parts. The first part describes the theoretical calculations on charmonium production cross sections in proton and ion induced collisions in the FAIR energy domain. For this purpose, we have adopted and adapted the originally proposed two component QVZ model. The model describes the J/ψ production in hadronic collisions as a factorizable two step process: (i) the production of the cc-bar pairs which involves a short time scale and can be accounted by perturbative QCD (pQCD) (ii) formation of the J/ψ mesons from the initially produced cc-bar pairs which is non-perturbative in nature and can be conveniently parametrized following existing prescriptions of colour neutralization. In case of p+A and A+A collisions the model takes into account for both initial state modification of the parton distribution functions inside the nucleus (nPDF) and final state dissociation of the produced pre-resonant cc-bar pairs with the prevailing cold nuclear matter. Before applying to the FAIR energy domain, the model is calibrated using the existing data on J/ψ production in p+A and A+A collisions at SPS energies. Model calibrated using the SPS data is then extrapolated to the FAIR energy domain to predict J/ψ suppression at FAIR energies. Model calculations indicate a larger CNM suppression at FAIR energies. The second part describes the simulational results on the optimization of a Muon Chamber (MUCH) detector system, for the Compressed Baryonic Matter (CBM) experiment at FAIR, for J/ψ detection via di-muon decay channel. Optimization studies are performed for the worst possible detection scenario i.e. central Au+Au collisions at various energies. Results show

very good signal-to-background (S/B) ratio and di-muon mass resolution which indicate highly feasible detection.

Publications

A. Refereed Journals:

1. Participation in the compressed baryonic matter experiment at FAIR S. Chattopadhyay, Y. P. Viyogi, P. P. Bhaduri and A. K. Dubey Published in Current Science Volume 100 No: 10 (2011)
2. J/yproduction in proton induced collisions at FAIR
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3. J/y suppression in a dense baryonic medium
   Partha Pratim Bhaduri, A.K. Chaudhuri and Subhasis Chattopadhyay Published in Phys. Rev. C 85, 064911, 2012 e-Print: arXiv:1206.0822 [hep-ph]
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B. Book Chapter(s):

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   Partha P. Bhaduri, Prasad Hedge, Helmut Satz and Prithwish Tribedy Published in Lect.Notes Phys.785:179-197, 2010. e-Print: arXiv:0812.3856 [hep-ph]

C. Conference proceedings:

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3. Differential elliptic flow & NCQ scaling of identified hadrons at FAIR energies Partha Pratim Bhaduri and Subhasis Chattopadhyay
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7. Di-muon measurements in CBM experiment at FAIR.

A. Prakash, P. P. Bhaduri, S. Chattopadhyay, A. Dubey and B.K. Singh Proceedings of ICPAQGP-2010, Goa, India Published in Nucl.Phys. A862-863 (2011) 493-496 e-Print: arXiv:1102.0882 [nucl-ex]

8. Sector layout of muon chambers (MUCH): first results
   Subhasis Chattopadhyay , Partha Pratim Bhaduri, Zubayer Ahammed and Arun Prakash
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10. Charmonium suppression in a baryon-rich quark-gluon plasma Partha Pratim Bhaduri, A. K. Chaudhuri and Subhasis Chattopadhyay Published in Page No: 696, Proceedings of the DAE SYMPOSIUM ON NUCLEAR PHYSICS, Volume 58 (2013)
11. Parton shadowing and J/psi suppression in nuclear collisions at SPS energy regime
    Partha Pratim Bhaduri, A. K. Chaudhuri and Subhasis Chattopadhyay Published in Page No: 718, Proceedings of the DAE SYMPOSIUM ON NUCLEAR PHYSICS, Volume 58 (2013)

D. Technical Reports

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2. Much layout optimization for SIS-100
   P. P. Bhaduri, A. Prakash and S. Chattopadhyay,
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3. Segmentation optimization for the MUCH detector
   A. Prakash, P. P. Bhaduri, B. K. Singh and S. Chattopadhyay,
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4. Sector layout of Muon Chambers (MUCH): First results
   S. Chattopadhyay, P. P. Bhaduri, Z. Ahammed and A. Prakash Published in CBM Progress Report 2010, Darmstadt 2011, p. 43
5. J/ty detection via di-muon channel in the CBM experiment at FAIR Partha Pratim Bhaduri and Subhasis Chattopadhyay Published in CBM Progress Report 2013, Darmstadt 2014, p. 117
6. Estimation of J/ty multiplicity in the CBM Experiment at FAIR Partha Pratim Bhaduri and Subhasis Chattopadhyay Published in CBM Progress Report 2013, Darmstadt 2014, p. 126

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Title	:	Design, Development and Characterization of High Current Electron Cyclotron Resonance Ion Source

Abstract

A high current Electron Cyclotron Resonance (ECR) proton ion source has been designed, fabricated, assembled, tested, characterized and commissioned for Low Energy high Intensity Proton Accelerator (LEHIPA) at BARC. The key components of ECR proton ion source that were designed and developed are the following: microwave generator and transmission system, plasma chamber, vacuum system, solenoid coils and power supplies, beam extraction electrodes and power supplies, gas injection system, beam and plasma measuring device and Low Conductivity Process Water system (LCW).

The ECR plasma generation, stabilization and characterization were performed before extracting the ion beam. An automated Langmuir probe and associated circuits were developed to characterize ECR plasma. The measured value of plasma parameters were in the range, ion density: 5.6 X10 cm" to 3.8 X10 cm^{-}, electron temperature: 4 eV - 14 eV and plasma potential: 20 V - 45 V. The studies were performed on the dependence of plasma parameters on neutral gas pressure, microwave power and radial location of the probe.

The characterization of the ion beam was performed in terms of total beam current, beam emittance and proton fraction. The total ion beam current of 40 mA (all species) was extracted at beam energy of 40 keV. The dependence of beam current on extraction voltage, microwave power and residual gas pressure were studied.

A low energy beam transport line (LEBT) has been designed and developed for measuring two important beam parameters i.e., beam emittance and proton fraction. The ion beam emittance was measured at three locations (i) at the ion source end after beam extraction, (ii) after focusing the beam using one solenoid magnet and (iii) after analyzing magnet.

The value of beam rms normalized emittance s_n measured for the above three cases falls in the range (i) 0.07 - 0.19 n mm-mrad (ii) 0.15 - 0.25 n mm-mrad and (iii) 0.02 - 0.11n mm-mrad respectively.

The proton fraction of the beam was measured by sweeping the magnetic field of the analyzing magnet and recording the current signal on a Faraday cup. The proton fraction measured was > 90%. The variation of proton fraction with microwave power and residual gas pressure were studied.

Publications

I. INTERNATIONAL REFFERED JOURNALS

a. Published

1. 'Beam Extraction and High Stability Operation of High Current Electron Cyclotron Resonance Proton Ion Source', P. Roychowdhury, L. Mishra, H. Kewlani, D. S. Patil and K. C. Mittal, Review of Scientific Instruments 85, (2014), p. 033303-1 to 033303-10.
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b. To be communicated

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II. ooks/Report/ General Articles

5. 'Design and Development of High Intensity ECR Proton Source for LEHIPA', P. Roychowdhury, BARC NEWSLETTER FOUNDER'S DAY Special Issue, October 2010, Paper No. 10.

III. CONFERENCE PROCEEDINGS

6. 'Development and Characterization of High Current Electron Cyclotron Resonance Proton Ion Source', P. Roychowdhury, L. Mishra, H. Kewlani, S. Grarat, D. S. Patil and K. C. Mittal, (Invited talk) Proceedings of Indian Particle Accelerator Conference, InPAC-2013, 19-21 November, 2013 VECC, Kolkata. p. 130, Paper No.: ITS-10.
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15. 'High intensity electron cyclotron resonance proton source development for LEHIPA', P. Roychowdhury, An Invited talk in Indo-Russian Meeting on linear Accelerators, IUAC, Delhi, 15 - 17 February 2010.
16. 'Simulation of ion beam extraction from single aperture triode extraction column', P. Roychowdhury and D. P. Chakravarthy, Proceedings of the International Symposium on Nuclear Physics, December 8-12, 2009, BARC, Mumbai, p.714.
17. 'High Intensity ECR Ion Source Development for LEHIPA-ADS-commissioning and operational experience', P. Roychowdhury, K. P. Dixit, S. R. Ghodke, P. C. Saroj, S. Chandan, S. Gharat, V. Yadav, R. B. Chavan and D. P. Chakravarthy, Proceedings of Indian Particle Accelerator Conference InPAC 2009, February 10-13, 2009, RRCAT, Indore, Paper No.226.

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Title	:	Perturbative and Non Perturbative Aspects of Lattice Quantum Chromodynamics

Abstract

The thesis studies both perturbative and non-perturbative aspects of lattice QCD. After introductions to the subjects of lattice QCD and fermion doubling, chapters three to eight contain new research findings. In chapters three and four, lattice QCD with unimproved Wilson fermion in the perturbative and non-perturbative QCD in the contexts of different branches of Wilson fermion and topological charge density correlator are studied. An extensive study of auto-correlation is performed in chapter five and chapter six introduces the concept of Wilson flow. Chapters seven and eight investigate topological susceptibility and scalar glueball in SU(3) Lattice Yang-Mills theory using Wilson flow employing both open and periodic boundary conditions''

Publications

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2. Title: "Topological susceptibility in lattice Yang-Mills theory with open boundary condition" Authors: Abhishek Chowdhury, A. Harindranath (Saha Inst.), Jyotir- moy Maiti (Barasat Govt. Coll.), Pushan Majumdar (IACS, Kolkata) Journal: Journal of High Energy Physics (JHEP) DOI: 10.1007/JHEP02(2014)045
3. Title: "Many avatars of the Wilson fermion: A perturbative analysis" Authors: Abhishe Chowdhury, A. Harindranath (Saha Inst.), Jyotir- moy Maiti (Barasat Govt. Coll.), Santanu Mondal (Saha Inst.). Journal: Journal of High Energy Physics (JHEP)
   DOI: 10.1007/JHEP02(2013)037
4. Title: "Exploring autocorrelations in two-flavour Wilson Lattice QCD using DD-HMC algorithm" Authors: Abhishek Chowdhury, Asit K. De, Sangita De Sarkar, A. Harindranath (Saha Inst.), Jyotirmoy Maiti (Barasat Govt. Coll.), Santanu Mondal, Anwesa Sarkar (Saha Inst.). Journal: Computer Physics Communications (CPC)
   DOI: 10.1016/j.cpc.2013.01.012
5. Title: "Topological charge density correlator in Lattice QCD with two flavours of unimproved Wilson fermions" Authors: Abhishek Chowdhury, Asit K. De, A. Harindranath (Saha Inst.), Jyotirmoy Maiti (Barasat Govt. Coll.), Santanu Mondal (Saha Inst.) Journal: Journal of High Energy Physics (JHEP) DOI: 10.1007/JHEP11(2012)029

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Abstract

The work in the thesis is focused on two main parts:

(i) the detailed simulation studies for the LEBT line for LEHIPA and measurements made on a LEBT test bench with helium, deuteron and proton beams and

(ii) Design studies for a 30 mA, 1 GeV proton linac.

The LEBT system is used to transport and match the beam from the ion source into the RFQ with minimum emittance growth and loss of beam current. The LEBT is also used to eliminate the unwanted ions like H_2+ and H_3+ from entering the RFQ. In addition, space charge compensation is required for transportation of such high beam currents. All this requires careful design and optimization. Detailed beam dynamics simulations were done to optimize the design of the LEBT using the PIC code TRACEWIN. It was found that with careful optimization it is possible to transport a 50 keV, 30 mA CW proton beam through the LEBT with 100% transmission and minimal emittance blow up, while at the same time suppressing unwanted species H_2+ and H_3+ to less than 3.3 % of the total beam current. The designed LEBT is 3.28 m long and its functions include beam focusing and steering at the RFQ match point, dc beam current diagnosis and beam profile measurement through CCD monitors. The design of various LEBT components like solenoid, steerer and electron trap was also done.

A LEBT was designed to match a 50 keV, 1 mA D+ beam into a 400 keV RFQ. Based on the simulations, a LEBT test bench was setup at Van de Graaff Laboratory to validate the simulations. The test bench consisted of an Alphatross ion source, Einzel lens, accelerating tube and 2 solenoids. He+, D+ and H+ beam were extracted from the ion source and accelerated to 50 keV. This 50 keV beam was then focused with the help of the 2 solenoids in the LEBT line. Experiments to measure the beam emittance of the beams in the line using solenoid scan method and slit wire method were done.

An accelerator configuration for a 1 GeV, 30 mA Linac has been worked out and the physics design studies have been done in detail. The front end consists of a 3 MeV RFQ, DTL upto 40 MeV and CCDTL upto 100 MeV while the high-energy Linac is made up of 5 cell superconducting elliptical cavities of 3 different types. The RFQ and DTL operate at 352.21 MHz and the CCDTL and SC Linac operate at the second harmonic frequency at 704.42 MHz. The transverse and longitudinal phase advances per unit length are maintained constant at all transitions between the structures to provide a current independent match into the next structure. For this, the quadrupole gradients and accelerating electric fields are varied between the structures. The design studies involved choice and optimization of various accelerating structures and the beam dynamics studies. The total length of the designed accelerator is about 380 m and the overall transmission is about 96%. The 4% loss takes place in RFQ during bunching of the beam which is not expected to pose any radiation problem.

In view of advances in the superconducting technology and new structures being developed for use in the medium energy range, it has now been planned to go for superconducting structures right after the RFQ for the 1 GeV linac for ADS. Two types of structures are now being considered as options for acceleration after the RFQ: the HWR at 162.5 MHz and the SSR at 325 MHz. The 3D electromagnetic designs for these structures have been done using CST Microwave Studio.

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Abstract

Fast reactors are one of the promising future energy options. Due to their breeding potential they could utilize a maximum quantity of uranium for energy production. Fast breeder reactors (FBR) have a compact core and have a large volumetric energy production rate. To extract large heat flux without significant increase in fuel and clad temperatures liquid sodium metal is used as the coolant due to the possibility of large heat transfer coefficient. Fuel pins in an FBR are housed in a hexagonal sheath and the pins are provided with helical wire-wrap. Also, the diameter of the fuel pin is small (3 – 6 mm) leading to small hydraulic diameter of the sub-channels. The fuel pin bundle, also known as subassembly, has a large number of tight sub-channels. Because of this, the inter-sub-channel communication is weak. This may have significant effect on the entrance flow characteristics in a subassembly. Further, the possibility of blockage formation within the subassembly and the attendant risk of local temperature increase are high. The present thesis attempts to investigate these aspects which are important in the design of a FBR core. For this purpose, three dimensional conservation equations of mass, momentum and energy are solved by using a finite volume based commercial computational fluid dynamics code employing appropriate turbulence models. The computational model is validated against published sodium experimental results in pipes, cylindrical annulus and rod bundles. Earlier research works were focused mainly on understanding the flow and temperature fields in the fully developed region. Large deviations were reported among published correlations for Nusselt number in pin bundles. Also, inter-play between blockage effects and developing flow / temperature fields has not been studied in the past. In the present work a detailed and systematic parametric study has been attempted. The parameters varied include the number of fuel pins, ligament gap, pin diameter, Reynolds number, helical wire-wrap pitch, ratio of triangular pitch to diameter of pins, blockage shapes, size, position and porosity.

Before attempting to study entrance flow in wire-wrap bundle the case of bare bundle is studied. During sodium flow through bare pin bundles development characteristics are seen to be strongly influenced by pin diameter, number of pins, ligament gap between the last row of pins and hexcan wall and Reynolds number. Flow development is achieved within an axial length of ~125 hydraulic diameters, for all the pin bundle configurations considered. But temperature development is attained only if the pin diameter is small or the number of pins is less. In the case of large pin diameter with more pins, temperature development is not be achieved even after a length of ~1000 hydraulic diameters. The reason for this behaviour is traced to be the weak communication among sub-channels in tightly packed bundles. It is seen that the pin Nusselt number decreases from centre to periphery in a bundle. Also, if the ligament gap is narrow, the Nusselt number is large and more uniform. Further, flow development length is short if the Reynolds number is large and the converse is true for thermal development length.

Following bare bundle study, investigation related to wire-wrap bundles has been carried out. During laminar flow through a wire-wrapped pin bundle, the friction factor is seen to exhibit a strong dependence on helical pitch where it increases as the pitch shortens. On the contrary, the Nusselt number does not exhibit such a strong dependence on helical pitch. A strong non-zero cross-stream velocity prevails in the fully developed region, contrary to that observed in straight channels. The mean value of non-dimensional cross-stream velocity is found to scale as $\pi D_r/H$, where, D_r is the pin diameter and H is the helical pitch of spacer wire. The friction factor and cross-stream velocity are relatively high in tight pin bundles.
In turbulent flow through helical wire-wrapped fuel pin bundle, the wire-wrap is found to promote a strong cross-stream velocity. It is found that the magnitude of mean cross-stream

velocity in the fully developed region is inversely proportional to the helical pitch length and it is nearly independent of the number of pins. Friction factor is seen to fluctuate periodically over a mean value and the fluctuation over each helical pitch corresponds to a specific position of helical wire. The mean value of the friction factor in the entrance region reduces below the mean value in the fully developed region contrary to that seen in ducted flows. Similarly, the Nusselt number passes through multiple minima before attaining fully developed periodic spatial fluctuations and its development is slower than that of friction factor. For a bundle with large number of pins the thermal development length is long. Traditionally, correlations reported for fully developed flow are considered for core design. But, the present study indicates that this approach may not be conservative. Further, the entrance region effects and the oscillations in the fully developed region have to be properly accounted in the core design. Based on the parametric study a correlation for Nusselt number is proposed as a function of helical pitch and other influencing parameters. The hotspot factor in the pin bundle is found to vary from 3 to 4. Further, it is large, either if Reynolds number is low or the number of pins is more.

In the last part of the research, sodium flow through fuel pin bundles with local blockage is investigated. For this, flow and temperature fields within a 19-pin wire-wrapped fuel bundle with internal blockage have been predicted. Simulations are carried out for a stream-wise length of 7 helical pitches. Clad temperature, cross-stream sodium velocity and cross-stream temperature distributions are investigated in detail. Axial distribution of clad temperature is seen to exhibit strong spatial variations due to the interaction of helical spacer wire and coolant flow through a subassembly with porous blockage. The maximum difference in the circumferential temperature of clad, which is a critical parameter for fuel pin mechanical design, is large in pins that are partially exposed to blockage. Effect of porous blockage is found to be limited to the porous zone and the peak clad temperature is proportional to the volume of the porous zone. Peak temperature in the blockage is strongly influenced by the radial extent of blockage and it is higher if the radial extent is larger. Maximum difference in the circumferential clad temperature is relatively low for a corner blockage compared to that of a central blockage. Sodium boiling is imminent in fuel pin bundle with six blocked sub-channels located at the centre when porosity value reduces below ~45%.

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Title	:	Liouville Fields, Mahler Fields and Schanuel's Conjecture

Abstract

In this thesis, we investigate some of the algebraic properties satisfied by Liouville numbers, and Mahler U-numbers. These are transcendental numbers which are very well approximated by algebraic numbers of bounded degree. We divide the thesis into four chapters.
Recall that, a real number <f is a Liouville number if, for each positive integer n, there exist positive integers p_n and q_n with $q_n > 2$ such that

|| SPn ||<C[n^n (1)

Here for any real number x we denote by | |x| | = $\min_{nez}$ \x - n|, the distance of x to the nearest integer.

The starting point of the first chapter is the elegant paper by Erdos: Every real number can be written as a sum of two Liouville numbers. Equivalently, for any real number t there are Liouville numbers x and y such that P{x, y) = 0, where P(x,y) = x + y — t. One of the proofs given by Erdos uses Bair's category theorem (G_s — subsets in a complete metric spaces are dense), and the fact that the collection L of Liouville numbers is a G§ — subset subset of R (the set of real numbers). Subsequent results were obtained by various authors.

We extend these results to a large class of functions, the so-called: Nowhere locally constant continuous functions. This class includes most of the polynomial functions, including the one P{x,y) = x + y — t for any real number t (from which the Erdos result follows).
In the second chapter, we introduce two new notions: Liouville sets and Liouville fields. These notions having their origin in the works of Maillet, a French mathematician. The Liouville sets are generalization of Liouville numbers. (Indeed, a real number £ is a Liouville number if and only if the singleton set {£} is a Liouville set. This happens if and only if the field generated by t, over Q, the field of rational number, is a Liouville field.) More precisely, Liouville sets are subsets of L whose elements have similar approximation of the form (1) for a fixed strictly increasing sequence q = $(q_{„})_n$>i of positive integers. We denote by S_q, theLiouville set corresponding to the sequence q of positive integers. In Theorem 2.4.1 we prove G3K an interesting fact that Q US_q is a field, for each q. We also prove that the sets S_q are either empty, or else uncountable. We characterize all such sets. Finally, we study some results concerning Liouville sets corresponds to inclusion and concatenation of the parameters q.

In the third chapter, we generalize the results obtained in the second chapter to the so-called Mahler sets and Mahler fields. Here, we consider some special subsets of the set U of Mahler's U — numbers, which have approximations in a fixed algebraic number field
(finite field extensions of Q) K . These sets are parameterized by (K,q), and we denote the Mahler set corresponding to (K, q^j by S_{Kq}. (The sets S_q corresponds to K = Q.) Like the sets S_q, the sets $S_{K\,q}$ have the following property, namely: K U$S_{K\,q}$ is a field. For each sequence q, the subfields of K U$S_{Ki\,q}$ are called Mahler fields over K. We completely

classify finite extensions of Mahler fields. We study quadratic extensions of some Liouville fields. We also prove some results about images of elements in Mahler fields under some special power series (which also includes the classical exponential function).

In the last chapter, we prove some results connected to the famous Schanuel's conjecture which states that: Given n > 1 number of Q — linearly independent complex numbers x_{lt} x_2,..., x_n, the transcendence degree of the field Q(x_v x_2,..., x_n, e^{Xl}, e^{X2},..., e^{Xn}) over Q is at least n. We show that, for any positive integers m, n with 1 < m < n, there exists uncountably many n -tuples ($£_{1(}$ Z;$_2$,..., $£_n$) of Liouville numbers such that ($£_{1(}$ <f_2-..., <f_n) are Q — linearly independent, e^' is a Liouville number for i = 1,2,..., n, and the transcendence degree over Q of the field Qtfx, %$_2$,..., $£_n$, e^^{1}, e^^{2},..., e^^{n}) = m + n. We also generalize this result to Mahler's U — numbers.

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2. Accepted.: K. Senthil Kumar. R. Thangadurai and M. Waldschmidt. Liouville Numbers, Liouville Sets and Liouville Fields, To appear in: Prof:. Arner. Math. Sac.
3. Communicated: K. Senthil Kumar. Fields of Mahlers U-mimbers, Preprint (2014).

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Title	:	Patterning of Si Surface by Medium Energy Ion Beam

Abstract

Self-organized processing of surface nanostructure has attracted interest due to promising applications of patterned surfaces as templates for deposition of functional thin films. Length scale associated with the nanostructure are reported to be varying with incident ion energy. A systematic study of medium energy ion induced pattern evolution, with particular attention to the features which remains unexplored till now, like classification of different temporal regime of evolution,processes contributing to pattern formation and the role of energy lossprocess etc., is still lacking.

In this thesis, we present our experimental investigations on medium energyAr^+ and Xe^+ion-beam induced morphological evolution ofp-Si(100) surface and related modifications in Si microstructure by employing characterization techniques like atomic force microscopy (AFM), cross-section transmission electron microscopy (XTEM), micro-Raman Spectroscopy, Rutherford backscattering spectrometry (RBS), and energy dispersive X-ray spectroscopy (EDS). In our studies, we have particularly addressed above mentioned important aspects of ion-beam patterning in this energy regime. In parallel to the experimental studies, we have carried out detail numerical estimations based upon current theoretical models of ion-bombarded surface evolutions which reveal that both the curvature dependent sputtering yield and atomic redistribution are responsible for pattern formation. Moreover, initial surface condition were found to be crucial for early stage of pattern formation. With the help of microstructural analysis, nuclear energy loss (being dominant over electronic energy loss)is found to be responsible for ion beam driven pattern formation. Statistical analysis of those generated ripple pattern shows the increasing nature in anisotropy as function of ion incident angle and ion fluence. This increasing anisotropic nature of ripple pattern also introduce the anisotropy in wettability of ripple pattern which is found to be increases with ion fluence. This behavior of wetting property wereunderstood in terms of physiochemical condition of the pattern surfaces.

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To be communicated

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Title	:	Studies with a Beta Particle Emitting Radionuclide in the Context of Radioimmunotherapy

Abstract

Radionuclides therapy is one of the therapeutic modalities of cancer, most often accomplished using radioisotopes capable of emitting alpha, beta and/or auger to deliver radiation dose to the target tissue, while sparing the neighboring healthy tissues. Biological effects of beta radiation are limited in literature. In this thesis ^{131}I has been used as a source for the beta radiation and effects on the human cancer cell lines were studied and were compared with an equivalent dose of γ-rays. To enhance the targeted delivery of beta radiation, ^{131}I was tagged with the rituximab (anti CD20 antibody), cell toxicity and underlying mechanism for the same was studied in CD20 expressing Raji cells. Additionally, the ^{131}I tagged rituximab was combined with conventionally used chemotherapy drug such as doxorubicin and mechanism of cell toxicity were also explored, for better understanding of therapeutic outcome. It was found that beta radiation emitted from radionuclide is more potent in induction of cell toxicity in tumor cells compared to the equivalent dose of γ radiation. RAD51 and P21 genes seem to have major role in discriminating the effect of beta and gamma radiation in Raji tumor cells. Effectiveness of tumor cell killing by ^{131}I increased after tagging with the rituximab and further enhanced by combining with doxorubicin. This increase in Raji cell death/apoptosis corresponds to the amount of cellular internalization of the ^{131}I-rituximab, which involves regulation by bclxl and the MAPK signaling pathways.

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Title	:	A Study on the Role of Thermokinetic Measurements and Modelling in Materials Design

Abstract

This synopsis describes in nutshell, the genesis, scope and organization of various components of this study. The importance of thermodynamic and kinetic investigations in facilitating the knowledge driven design of materials is exemplified by taking two case study materials. The comprehensive metallurgical aspects of high temperature phase stability of an indigenous variety of reduced activation ferritic-martensitic steel are investigated using isothermal drop and dynamic scanning calorimetry. Highly accurate experimental estimates of both energetic and kinetic quantities of α-ferrite+carbide$\rightarrow\gamma$-austenite phase transformation have been obtained. The systematics of martensite formation upon cooling from high temperature γ-austenite phase has been extensively probed. Further, drop calorimetry based values of enthalpy and heat capacity, and their variation with temperature have been presented, probably for the first time for any RAFM steel.

In case of Ferroboron, a novel and economical shielding candidate for future Indian fast reactors, the high temperature thermal stability, thermal properties, such as heat capacity and anisotropic lattice expansion and its metallurgical compatibility with SS 304L clad etc., have been characterized, again by a combination of calorimetry, metallography and modelling.

In addition, a rigorous thermodynamic analysis of the interrelationship between various thermodynamic quantities, such as molar volume, enthalpy, entropy and bulk modulus has been presented. The potential use of such a thermodynamic modelling apparatus is illustrated by presenting a comprehensive assessment of thermophysical data of α-Pu, a highly radioactive element. In a similar vein, a critical appraisal of various popular models of diffusional solid state transformations has been made, and a proposal for the consistent physically based analysis of the role of heating and cooling rates in altering the kinetics, has been presented.

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5. S. Raju and E. Mohandas, Kinetics of solid state phase transformations: Measurement and Modelling of some basic Issues, J. Chem. Sci., 2010, 122, 83-89.
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Name	:	**Rajesh Kumar**
Enrolment No.	:	PHYS01200804017
Date of Award of degree	:	23.12.14
Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	Development of Methods for Dosimetry Quality Assurance in Intensity Modulated Radiation Therapy/Image Guided Radiation Therapy (IMRT/IGRT)

Abstract

The candidate has carried out comprehensive studies on patient specific IMRT QA in India by conducting national survey on IMRT QA using a well structured questionnaire, multi-centre patient specific IMRT dosimetric inter-comparison by on-site visit and analysis of pre-treatment dosimetric QA result of different hospitals. It was found that there is a requirement of national protocol for IMRT QA so that treatment outcomes of all the IMRT centers of country can be compared. It was also pointed that dosimetry quality audit prior to commissioning of IMRT may play an important role in eliminating discrepancies in IMRT commissioning at beginning itself. Further, As per the special requirement of IMRT, candidate has developed a novel and low cost phantom for dosimetry QA in IMRT as import substitute. Its efficacy was also compared with commercial system. For establishing dosimetry audit program for IMRT, methodology and a portable phantom simulating thorax region were developed and a trail study was conducted.

Measurement based patient specific IMRT QA is performed only for limited number of times and require considerable time of delivery system as well as of medical physicist. However, catastrophic type of errors can occur at any time during the course of treatment. If the treatment planning system has been commissioned suitably for IMRT and adequate periodic machine QA for IMRT are in place, measurement based patient specific IMRT QA can be replaced with software based IMRT QA. In this connection, methodology was evolved to compare leaf positions as measured from EPID images for IMRT treatment to the data in the Log/Trajectory files and use

them as tools for quick, efficient and effective patient specific IMRT QA.

He has also carried out volumetric dose verification using dose at 98%, 95%, 2% volume of interest and 3D gamma analysis methods by incorporating quantitative 3D gamma analysis tools in Computational Environment for Radiotherapy Research software.
A dynamic phantom for QA in 4D radiotherapy was designed, fabricated and its suitability in 4DRT was demonstrated.

Publications

Journal

1. Rajesh Kumar, S.D. Sharma, Sudesh Despande, Yogesh Ghadi, V.S. Shaiju , H.I. Amols and Y. S. Mayya. “Acrylonitrile Butadiene Styrene (ABS) plastic-based low cost tissue equivalent phantom for verification dosimetry in IMRT". J Appl Clin Med Phys., 17;11(1):3030. (2009)
2. Kumar R, Sharma S.D, Amols H.I., Mayya Y.S. and Kushwaha H. S. “A Survey on the Quality Assurance Procedures Used in Intensity Modulated Radiation Therapy (IMRT) at Indian Hospitals”. J Cancer Sci Ther, 2: 166-170(2010)
3. Deshpande S, Kumar R., Ghadi, Y., Neharu, R.M., Kannan, V. “Dosimetry Investigation of MOSFET for Clinical IMRT Dose Verification” Technol Cancer Res Treat 12, 193-198 (2013)
4. Kumar R, Sharma S D, Deshpande S, Sresty N M, Bhatt C P, Amols HI, Chourasiya G, Mayya Y S. “Analysis of patient specific dosimetry quality assurance measurements in intensity modulated radiotherapy: A multi centre study.” J Can Res Ther 2014;10:611-7

Communicated

1. Rajesh Kumar, C.P.Bhatt, S.D.Sharma, G.Chourasiya, D.A.R.Babu, J.Singh, A.Apte, H.I.Amols and Y.S. Mayya. “Three Dimensional Gamma Analysis in Volumetric Dose Verification in Intensity Modulated Radiation Therapy " Medical Dosimetry

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2. Rajesh Kumar, S. D. Sharma, S. Deshpande, K. Thakur, S. Patkar, G Chourasiya and D.A.R. Babu. “A Portable IMRT Dosimetry Quality Audit phantom” Souvenir andAbstract Book, National Conference of Association of Medical Physicists of India. Kolkata, November 13-16,2013 Pp 144-145
3. Rajesh Kumar, S.D. Sharma, Suresh Choudhari, Yogesh Ghadi , D.D. Deshpande, G. Chourasiya . “Dosimetry Studies using different type of IMRTPhantoms”. J. Med. Phys. Book of Abstract AMPICON-2010 Special Issue-JMP(2010), pp 68
4. Sudesh Deshpande, Rajesh Kumar, S.D. Sharma, Parimal Patwe, Ritesh Mahatre “IMRT dosimetric studies as per AAPM TG119 Suits”, J. Med. Phys. Book of Abstract, AMPICON-2010 Special Issue-JMP (2010), Pp 30
5. Rajesh Kumar, S D Sharma, S. Deshpande, Y. Ghadi and Y S Mayya. “Patient specific dosimetric verification in IMRT using indigenously developed low cost tissue equivalent phantom”. Souvenir and Abstract Book, International Conference on Medical Physics, Mumbai, November 26-29, 2008.
6. Rajesh Kumar, C.P.Bhatt, S.D.Sharma, G.Chourasiya, D.A.R.Babu, J.Singh, A.Apte, H.I.Amols and Y.S. Mayya. “Gamma Analysis in Volumetric Dose Verification in Intensity Modulated Radiation Therapy”. Indian Association for Radiation Protection National Conference (IARPNC-2014), Mumbai. March 19-21, 2014

Name	:	**Sumanta Pal**
Enrolment No.	:	PHYS01200804031
Date of Award of degree	:	23.12.14
Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	Development of the INO-ICAL Detector and its Physics Potential

Abstract

In the world wide endeavour of the precision study of the neutrino parameters Indian scientists are also making contributions building the magnetised neutrino detector, the Iron CALorimeter (ICAL) with Resistive Plate Chambers (RPCs) as its active detector elements, at the proposed India based Neutrino Observatory (INO) site. The ICALdetector is tuned to detect mainly muons coming from atmospheric neutrinos. ICAL will have a good tracking, momentumand time resolutions alongwith the charge identificationcapability. With these capabilities, ICALwill look for precisionmeasurementsof neutrino oscillation parameters and determine the neutrino mass ordering. The performanceof the detector as per the expectation and in parallel confident understandingof various signals in the detector through physics simulation studies play a key role inachieving the physics goal.

Successful completion of designing, building and characterising large size RPCshave already beendone. To continue this development, detailedstudy of muon tracking efficiencies by RPCs, detailed study of time resolutions of theRPCs along with a scheme for time calibration for each RPC was taken up and is reportedin the first part of the thesis. These calibrations are then used to study thecosmic muon flux on the Earth's surface and their directionality in the prototype RPCstack at TIFR, Mumbai. Such cosmic muons form major background to the study ofatmospheric neutrinos which is the main focus of ICAL.

Atmospheric neutrinos contain only muonand electron-type neutrinos. At sufficiently long distances, oscillations of muon-type neutrinos to tau-typeneutrinos are dominant due to the large relevant mixing angle, θ_{23}. Therecent confirmation of large value of θ_{13} alsoenhances oscillations of electron-type neutrinosto tau-type neutrinos. Hence tau neutrinos (and anti-neutrinos) are expectedto be copiously produced when atmospheric neutrinos pass through the Earth andreach the detector. These tau neutrinos will undergo charged-current (CC) interactions,while interacting with the target material of the ICAL detector, to producecharged tau leptons in the detector. Decay product of these tau leptons, mainly hadrons contaminate the neutral current (NC) sample of atmospheric neutrinos. In the precisionstudy of neutrino oscillation parameters, effects of any contaminated signal tothe main signal can crucially alter the result. In view of that, a detailed study of taudecays to hadrons are reported in the second part of the thesis.

Publications

Peer-reviewed research papers:

1. Measurement of integrated flux of cosmic muons at sea level using the INO-ICAL prototype detector, S. Pal, B. S. Acharya, G. Majumder, N .K. Mondal, D. Samuel and B. Satyanarayana, Journal of Cosmology and Astroparticle Physics, JCAP07,2012, 033.
2. Study of the directionality of cosmic muons using the INO-ICAL prototype detector, S. Pal, G. Majumder, N .K. Mondal, D. Samuel and B. Satyanarayana, Nuclear Instrumentation and Methods in Physics Research SectionA:Accelerators, Spectrometers, Detectors and Associated Equipment, 735, 2014, 88–93.
3. Preliminary results on optimisation of gas flow rate for ICAL RPCs, B. Satyanarayana, S. Pal,M. R. Bhuyan, S.D. Kalmani,N. K.Mondal and R. R. Shinde, Nuclear Instrumentation and Methods in Physics Research Section
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Conference proceedings:

1. Measurement of integrated flux of cosmic muons at sea level using the India-based Neutrino Observatory prototype detector, S. Pal, G. Majumder, N .K. Mondal, D. Samuel and B. Satyanarayana, Proceedings of Science (PoS-RPC2012) 021.
2. Angular distribution of cosmic muons using INOICAL prototype detector atTIFR, S. Pal, G. Majumder, N .K. Mondal, D. Samuel and B. Satyanarayana, PRAMANA - journal of physics, November 2012, Volume 79, Issue 5, pp 1267-1270.
3. Velocity measurement of cosmic muons using the India-based Neutrino Observatory prototype detector, S. Pal, G. Majumder, N .K. Mondal, D. Samuel and B. Satyanarayana, Nuclear Instrumentation and Methods in Physics Research SectionA: Accelerators, Spectrometers, Detectors and Associated Equipment, 661,2012, S77.

Others:

1. Cosmic ray test of INO RPC stack, M. Bhuyan, V. M. Datar, S. D. Kalmani, S. M. Lahamge, N. K. Mondal, P. Nagaraj,S. Pal, L. V. Reddy, A. Redij, D. Samuel, M. N. Saraf, B. Satyanarayana,R. R. Shinde, P. Verma, Nuclear Instrumentation and Methods in Physics Research SectionA: Accelerators, Spectrometers, Detectors and Associated Equipment, 661, 2012, S68.
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To be published:

1. Simulation study of tau induced hadron events in the ICAL detector. D. Indumathi and S. Pal.

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Date of Award of degree	:	30.12.14
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Title	:	Cloning and Characterization of Three Abiotic Stress Related Genes (Dehydrin, WRKY and bZIP) and their Overexpression in Bananna

Abstract

Plant growth and development are adversely affected by different abiotic and biotic stress factors. Plants respond to these stresses by employing specialized physiological and biochemical strategies. Upon stress perception, plants trigger a cascade of cellular events involving several parallel transduction pathways that eventually modulate the level of specific transcription factors resulting finally in the up or down regulation of genes coding for synthesis of effector proteins and/ or metabolites which participate in stress tolerance. Banana (Musa spp.) is one of the most important food and fruit crops in the world. India is the highest producer of bananas in the world with a total production of 31.89 million metric tones, which is approx. 34.5 % of total production of top 20 banana growing countries. As part of this doctoral study, three banana abiotic stress related genes (Dehydrin, WRKY and bZIP) were cloned and characterized by their overexpression in transgenic banana plants. Dehydrins are highly hydrophilic proteins involved in playing key adaptive roles in response to abiotic stress conditions having dehydration as a common component. A novel banana SK_3-type dehydrin, MusaDHN-1, was identified and characterized using transgenic banana plants. Expression profiling in native banana plants demonstrated that

MusaDHN-1 was induced in response to varied abiotic and biotic stress mimics. Transgenic banana plants constitutively overexpressing MusaDHN-1 displayed improved tolerance to drought and salt-stress treatments in both in vitro and ex vitro assays. WRKY transcription factors are specifically involved in the transcriptional reprogramming following incidence of abiotic or biotic stress on plants. A novel WRKY gene from banana, MusaWRKY71, was identified in banana EST database and was found to be inducible in response to a wide array of abiotic or biotic stress stimuli. The MusaWRKY71 gene was overexpressed in transgenic banana plants. Stable integration and overexpression of MusaWRKY71 in transgenic banana plants was proved by Southern blot analysis and quantitative real time RT-PCR. Transgenic banana plants overexpressing MusaWRKY71 displayed enhanced tolerance towards oxidative and salt stress. Further, differential regulation of putative downstream genes of MusaWRKY71 was investigated using real-time RT-PCR expression analysis. bZIP transcription factors are involved in diverse cellular processes including stress response pathways in plants. A bZIP gene, MusabZIP53, was identified from banana EST database and subsequently characterized by overexpression in transgenic banana plants. Expression profiling in native banana plants proved that MusabZIP53 was strongly up-regulated by cold and drought stress and by ABA treatment in both leaf and root tissues. Transgenic banana plants constitutively overexpressing MusabZIP53 displayed growth retardation from early stages of transformation/regeneration protocol and mature greenhouse hardened transgenic plants displayed a distinct dwarf phenotype. Genes belonging to several families known to be involved in abiotic stress perception and mitigation were found to be differentially regulated in these transgenic plants. Among the three genes characterized in this study, the MusaDHN-1 dehydrin gene is the most suited to develop abiotic stress tolerant banana plants.

Publications

Journals

1. "Cloning and characterization of a novel stress-responsive WRKY transcription factor gene (MusaWRKY71) from Musa spp. cv. Karibale Monthan (ABB group) using transformed banana cells", Shekhawat UKS, Ganapathi TR, Srinivas L, 2011, Molecular Biology Reports 38, 4023-4035.
2. "MusaDHN-1, a novel multiple stress-inducible SK_3-type dehydrin gene, contributes affirmatively to drought- and salt-stress tolerance in banana" Shekhawat UKS, Ganapathi TR, Srinivas L , 2011, Planta 234, 915-932.
3. "MusaWRKY71 overexpression in banana plants leads to altered abiotic and biotic stress responses", Shekhawat UKS, Ganapathi TR, 2013, PLoS One, 8, e75506.
4. "Transgenic banana plants overexpressing MusabZIP53 display severe growth retardation with enhanced sucrose and polyphenol oxidase activity", Shekhawat UKS, Ganapathi TR, 2014, Plant Cell, Tissue and Organ Culture, 116, 387-402.

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1. "Overexpression of a native SK_3-type dehydrin enhances tolerance to drought and salt stressmin banana", Shekhawat UKS, Srinivas L, Ganapathi TR, 2011, National Symposium on Recent advances in plant tissue culture and biotechnological researches in India at M.N. Institute of Applied Sciences, Bikaner, 4-6 Feb.
2. "Characterization of MusaWRKY71, a multiple stress inducible WRKY gene using transgenic banana plants", Shekhawat UKS, Ganapathi TR, 2012, DAE BRNS Life Science symposium on "Trends in Plant, Agriculture and Food Sciences" at BARC, Mumbai, 17-19 Dec.

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1. "Studies on MusaWRKY71, a multiple stress inducible transcription factor gene from banana which is involved in diverse stress responses", Shekhawat UKS, Ganapathi TR, 2013, BARC Newsletter, Oct 2013.

Name : **Param Jeet Singh**
Enrolment No. : PHYS01201004011
Date of Award of degree : 03.01.15
Constituent Institute : Bhabha Atomir Research Centre, Mumbai
Title : Synchrotron Radiation Based VUV Spectroscopy of Some Polyatomic Molecules of Environmental Interest

Abstract

The studies presented in this thesis are concerned with VUV spectroscopic investigations of electronic states of molecules in gas-phase and in rare gas matrices in the wavelength range 1050-2500 A (5-11.8 eV, 40,000-95,240 cm^{-1}). Design and development of experimental systems for VUV spectroscopy, which include the HRVUV beamline and experimental stations for photoabsorption and matrix isolation spectroscopy are discussed. Gas phase photoabsorption studies of the E -X system of SO_2 in the 7.7-8.6 eV region is investigated and the electronic states involved in the E -X system and their symmetries are discussed with the help of vertical excited state calculations. A unified picture of the VUV spectroscopy of acetone-h_6 (CH_3COCH_3) and its deuterated counterpart acetone-d_6 (CD3COCD3) is presented. Extensive Rydberg series and vibronic features are assigned by taking into account the symmetry selection rules and contributions of hot bands from low lying torsional modes. Revised quantum defect values for the Rydberg transitions and a few new assignments are proposed. The Rydberg and vibronic investigation of the electronic spectra of chloroform (CHCl3) and its deuterated counterpart (CDCl3) in the energy region 6.2-11.8 eV is presented. Identification and analysis of Rydberg series converging to the first four IPs at 11.48, 11.91, 12.01 and 12.85 eV corresponding to excitation from the $1a_2$, 4a\, 4e, 3e orbitals of $CHCl_3$ respectively are presented. Analysis is aided by quantum chemical computations of excited states. Assignment of vibrational progressions to v_3' (CCl_3 s-deform) mode and combination modes of v_3' and v_6' (CCl_3 d-deform) belonging to $1a_2$^-4p transition is confirmed based on a study of the vibronic spectrum of $CDCl_3$. VUV spectra of SO_2 and acetone isolated in inert gas matrices at cryogenic temperatures are studied in order to understand better the nature of the excited states and their interactions in rare gas matrices. Electronic transitions observed in matrix isolated acetone show blue shifts of ~3000-6000 cm^{-1}, as expected for Rydberg transitions. In the case of SO_2, the first three absorption bands are not shifted much in the matrix phase as compared to the gas phase, whereas the higher excited states show larger shifts. This is in line with the assignment of the first three gas phase absorption systems to valence transitions, and higher bands to transitions of valence- Rydberg mixed or Rydberg character. Finally the important conclusions of the present studies and future directions of work are discussed.

Publications

Journal

1. “First commissioning results from high resolution vacuum ultraviolet beamline at indus-1 synchrotron source”, Param Jeet Singh, Aparna Shastri, R. Sampath Kumar, S.N. Jha, S.V.N. B. Rao, R. D’Souza and B.N. Jagatap, Nuclear Instruments and Methods in Physics Research-A, 2011, 634 113 - 119.
2. “VUV photoabsorption spectroscopy of Sulphur dioxide in the 1400 -1600 A region: vibronic analysis of the E - X system”, Param Jeet Singh, Aparna Shastri, R. D’Souza, S.V.N. B. Rao and B.N. Jagatap, J. Quant. Spectrosc. Radiat. Transf., 2012, 113, 267 - 278.
3. “The role of torsional modes in the electronic absorption spectrum of acetone”, Aparna Shastri, Param Jeet Singh, B.N. Raja Sekhar, R. D'Souza and B.N. Jagatap, J. Quant. Spectrosc. Radiat. Transf., 2012, 113, 1553 - 1565.
4. “Excited state vibrational modes of a few triatomic molecules of environmental interest”, Aparna Shastri, Sunanda K., Param Jeet Singh, B.N. Raja Sekhar, S.V.N. Bhaskar Rao, R. D’Souza and B.N. Jagatap, Asian Journal of spectroscopy, 2012, special issue, 107 - 119.
5. “Effect of isotopic substitution in the electronic absorption spectrum of acetone: VUV

photoabsorption studies of acetone-d_6", Param Jeet Singh, Aparna Shastri, B.N. Raja Sekhar, R. D'Souza, B.N. Jagatap, J. Quant. Spectrosc. Radiat. Transf., 2012, 114, 20 - 28.

6. "Rydberg states of chloroform studied by VUV photoabsorption spectroscopy", Param Jeet Singh, Aparna Shastri, R. D'Souza and B.N. Jagatap, J. Quant. Spectrosc. Radiat. Transf. 2013, 129 204 - 213.
7. "Development of an experimental set-up for low temperature spectroscopic studies of matrix isolated molecules and molecular ices", Param Jeet Singh, B.N. Raja Sekhar, K. Sundararajan, Aparna Shastri, Vijay Kumar, Anuvab Mandal, A.K. Sagar, M.S. Ansari, P.K. Kush, B.N. Jagatap, Nuclear Instruments and Methods in Physics Research-A, communicated.
8. "VUV photoabsorption spectrum of acetone isolated in argon matrix", Param Jeet Singh, Aparna Shastri, B.N. Raja Sekhar, K. Sundararajan, Vijay Kumar, B. N. Jagatap, Chemical physics, Communicated.

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2. "VUV Photoabsorption Studies of CHCl3 and CDCl3 Using photophysics Beamline at Indus-1" Aparna Shastri, Param Jeet Singh, B.N. Raja Sekhar and R. D'Souza, National symposium on radiation & Photochaemistry, JNV, Jodhpur, 2011.
3. "VUV Absorption Spectrum of the E-X System of SO2" Param Jeet Singh, Aparna Shastri, S.V.N. Bhaskara Rao and R. D'Souza, DAE-BRNS Symposium on Atomic, Molecular and Optics physics, Karnataka University, Dharwad, 2011.
4. "The role of torsional vibrations in the electronic absorption spectrum of acetone", Aparna Shastri, B.N. Raja Sekhar, Param Jeet Singh, 99th Indian Science Congress, KIIT University, Bhubaneswar, 2012.
5. "VUV spectroscopy of SO2 isolated in argon matrix using synchrotron radiation", Param Jeet Singh, B.N. Raja Sekhar, V. Kumar, A. Mandal, Aparna Shastri and B.N. Jagatap. DAE-BRNS Symposium on Atomic, Molecular & Optical Physics-AMOP-2012, IISER, Kolkata, 2012.
6. "Synchrotron based VUV spectroscopy in gas and matrix isolated phase" Param Jeet Singh, Anuvab Mandal, Vijay Kumar, A. Shastri, B.N. Raja Sekhar, B.N. Jagatap, The 7th Asia Oceania Forum for Synchrotron Radiation Research, Egret, Himeji, Japan, 2013.

Others (Invited Talk)

1. "VUV Spectroscopy of Environmentally Important Molecules in Gas Phase and Matrix Isolated Phase Using Synchrotron Radiation" Param Jeet Singh, Anuvab Mandal, Vijay Kumar, Aparna Shastri, K. Sundararajan, B.N. Raja Sekhar and B.N. Jagatap, National Symposium on Radiation and Photochemistry, North East Hill University, Shillong, 2013.

Name	:	**K.K. Kuriakose**
Enrolment No.	:	STRA02200704001
Date of Award of degree	:	07.01.15
Constituent Institute	:	Indira Gandhi Centre for Atomic Research, Kalpakkam
Title	:	Information Technology and Knowledge Engineering Centric Knowledge Management: A Maturity Model Based on Key Maturity Indicators

Abstract

Knowledge management (KM) aims to create wealth and value by providing organisational entities, the right knowledge, at the right place and at the right time. KM has proven benefits and has been adopted by 80% of the world's biggest companies. Knowledge management maturity model describes the development of KM over time. It provides a roadmap for successful KM implementation. The objective of the thesis is to develop a flexible and adaptable KM maturity model and demonstrate its utility in the context of a government controlled nuclear research and development (R&D) organisation. This model is the core contribution of this thesis to the literature in KM. Vast amount of nuclear knowledge has been created and accumulated through decades of R&D and operational experience. This knowledge is of paramount importance for the continued use of existing nuclear installations and future innovations. Unfortunately the present status of nuclear knowledge and its management still remain in an unsatisfactory condition. It is in this organisational context that the development of a KM maturity model was undertaken.

The thesis presents a detailed review of KM literature covering various facets such as people, process, technology, knowledge and return on investment. Detailed study of the existing KM maturity models and the morphological analysis carried out is discussed. The context of the nuclear R&D organisation, where the knowledge management maturity model was demonstrated, is discussed. A new KM maturity model, viz. KMI-KMM proposed is discussed. The model is validated by expert judgment. The application and validation of this model through a case study is discussed. The maturity level of the organisation and its 10 groups were assessed, through the case study. The inhibiting factors of the organisation and its groups were identified through a survey. Flexibility of the proposed model and its adaptability to other organizations have been demonstrated. The process of knowledge creation and 'ba' in the context of one group of the organisation was studied. A taxonomy pertaining to the knowledge of one group was developed. The conclusions, contributions, recommendations and scope for further work are discussed.

Publications

Journal

1. "Assessment of Knowledge Management Maturity in an R&D Organization", K.K.Kuriakose, Baldev Raj, R.Malathi, V.Parameswaran, S.A.V.Satya Murty , Journal of Knowledge Management Practice, December, 2011, Vol 12. No 4, available at www.tlainc.com/articl283.htm
2. "Knowledge Management Maturity Model: An Engineering Approach" K.K. Kuriakose, Baldev Raj, S.A.V. Satya Murty and P. Swaminathan, Journal of Knowledge Management Practice, June, 2011, Vol 12, No.2, available at www.tlainc.com/articl263.htm
3. "Knowledge Management in Fast Reactors" K.K. Kuriakose, S.A.V. Satya Murty, P. Swaminathan and Baldev Raj, Elsevier Energy Procedia , Vol 7, 2011, 672-677.
4. "Knowledge Management Maturity Models –A Morphological Analysis" K.K. Kuriakose, Baldev Raj, S.A.V. Satya Murty and P. Swaminathan, Journal of Knowledge Management Practice, September,2010, Vol 11, No.3, available at www.tlainc.com/articl232.htm

Conferences

1. "The Role of Ba in Knowledge Creation and Innovation in the Context of an R&D Organization", K.K.Kuriakose, R. Malathi, V.Parameswaran, and S.A.V. Satya Murty, Proceedings of 8th National Conference on Recent Advances in Information Technology-READIT 2011, 28-29, December 2011, Kalpakkam, 82-89.
2. "Knowledge Management, Knowledge Sharing and Co-opetition-A Case Study" K.K. Kuriakose, R. Malathi, V. Parameswaran, S.A.V. Satya Murty and P. Swaminathan, Proceedings of 7th National Conference on Recent Advances in Information Science and Technology- READIT 2009, 29-30 Dec. 2009, Kalpakkam, 145-152.

Name	:	**Rohit Shukla**
Enrolment No.	:	PHYS01200804007
Date of Award of degree	:	14.01.15
Constituent Institute	:	Bhabha Atomir Research Centre, Mumbai
Title	:	Experimental Study on Optimum Space-Charge Effects and Enhanced Free-Space Coupling for Vircator Driven by Compact Driver

Abstract

Ultra compact PT charges the solid dielectric PFL in 2/j.s and 1µs made by RG218 cable and 450kV XLPE cable in the presented results. The achieved voltage gains of PT are 1:20 in such compact geometries. PFL are made of coaxial cable to drive electron beam diode in form of vircator and are reported for the first time. The microwave emission from such compact PFL charged by new-configuration PT is reported for 1MW radiation in frequency range of 4-8GHz. The vircator is operated with the help of dry PFL at repetition rate of 4Hz and consistency of results in terms of frequency and peak power upto six sequential shots is reported in the repetitive operating mode. Shot to shot variation is also shown to be very little in terms of frequency and peak radiated power in single shot mode of operation. The cable based PFL pulsed power generator has electrical peak power delivery of 650MW and 3.3GW respectively when they are made using RG218 cable in one case and high voltage XLPE cable in the other case. A broadband conical horn antenna to maximize the radiation at the axis of vircator is designed and implemented after the vircator. 3D modelling results if the antenna are also presented. The vircator efficiency of 0.3% is also reported and extensive modelling of the results in PIC code (XOOPIC two and half dimensional code) is also presented. The vircator is reported to be operating at 50kV of A-K gap voltage which is the lowest reported in conventional vircator geometry. At these low anode cathode voltages the current densities (computed assuming uniform emission) achieved are 300A/cm^2 which is quite close to the highest values reported in the literature i.e. 450A/cm^2. For single shot applications ultra compact pulsed power generators using exploding copper wire as opening switch is reported for 500MW and 2GW peak electrical power delivery capabilities in two reported cases. All the switches in this generator are in air and hence device is very attractive. The experimental, modelling results of these compact generators aimed for vircator as load is presented.

Publications

Published in Peer Reviewed Journals:

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2. Low voltage, low energy and repetitive (4Hz) operation of a conventional vir- cator for microwave emission in the range of 4-8 GHz R.Shukla, A. Shyam Laser and Particle Beams 31 Issue 04 pp 627-634 (2013)

3. Microwave Emission from a AXIAL-Virtual Cathode Oscillator Driven by Compact Pulsed Power Source R. Shukla, P.Bannerjee, S.K. Sharma, R. Das, P Deb, Prabaharan T., B.K. Das, B. Adhikary, R.Verma, A.Shyam Journal of Physics Conference Series (2012)
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Abstract

The sensitivity of a Cherenkov imaging telescope is strongly dependent on the rejection of the cosmic-ray background events. The conventionally used Supercuts/Dynamic Supercuts method, though using several image parameters simultaneously, ignores possible correlations among the parameters. One of the main objectives of the thesis is to study the gamma / hadron segregation potential of various ANN algorithms by applying them to the Monte Carlo simulated and actual observational data collected with TACTIC telescope. The results obtained suggest that Levenberg-Marquardt method outperforms all other methods in the ANN domain. Applying this ANN algorithm to ~101 h of Crab Nebula data collected by the TACTIC telescope, yields an excess of ~ (1141 ± 106) with a statistical significance of ~11.1 o, as against an excess of ~(928 ± 100) with a statistical significance of ~ 9.4 o obtained with Dynamic Supercuts selection methodology. The main advantage accruing from the ANN methodology is that it is more effective at higher energies and this has allowed us to re determine the Crab Nebula energy spectrum in the energy range 1-24 TeV. A novel energy reconstruction procedure, based on the utilization of ANN, has been also developed for the TACTIC telescope. The new ANN- based energy reconstruction method, apart from yielding an energy resolution of ~ 26%, which is comparable to that of other single imaging telescopes, has the added advantage that it considers zenith angle dependence as well.

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B.S.Sahayanathan, M.Sharma, C.K.Bhat, N.Bhatt, S.Bhattacharyya, C.Borwankar, M.K.Koul. Presented at " TeV Particle Astrophysics 2012 Mumbai, India,(2012).

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Title	:	Design and Developmental Aspects of High Power Ultra-Wideband 3DB Hybrid Coupler for ICRF Heating in Tokamak

Abstract

The ICRH system of tokamak utilizes ontinuous wave rf p ower ab ove 100kW and upto few MW at many frequen ies in the range of 20 to 120MHz. The frequeny depends up on geometry of the tokamak, desired plasma parameters and toroidal magnetic field at the enter of tokamak vessel. The ICRF generators are used to feed the rf power to the plasma with ICRH antennae. These should ideally be operated into mat hed load. The antennae load imp edan e not only dep ends on the antennae geometry but also on the boundary onditions of plasma which oer ontinuously variable mismatch. Due to the mismat hed loading, significant amount of the rf power is reted back and auses in onsitant performance or damage to the generator. The conventional matching systems operate on slower time s ale and may fails to cope with the faster variation of plasma impedance. The 3dB hybrid oupler is used to provide the essential prote tion to the rf generator from the repe ted p ower. The 3dB hybrid oupler an also be used as power combiner, divider and to prote t the rf sour e by oupling of ree ted p ower to the isolated port.

The 3dB hybrid coupler is a 4-p ort devi e in whi h input of rf power at port-1 is equally divided into the port-2 and port-3 with a phase difference of 90◦ , whereas port-4 is remain isolated. In case, ree ted p owers due to mismat hed load at port-2 and port-3 that are connected to antennae are equal in magnitude and phase, the total reflected power goes to p ort-4. Thus, rf generator is protected from reflected power. The high p ower hybrid ouplers that are developed and presently available for these purp oses are rated for narrow frequen y band and do not over full op erational frequen y range of the prop osed ICRH exp eriments. Many 3dB hybrid coupler, at various disrete frequen ies are required in the ICRF range. Therefore, hybrid oupler and the oupling me hanism needs to be altered with hange of operating frequeny. The development of broadband 3dB hybrid oupler in the high power rating is not yet reported. Therefore, the need is felt and the author is motivated to intensify his resear h interest in this domain. The work has b een ompleted in following steps:

1. A strip line based prototyp e 3dB tandem hybrid oupler of rating, 91.2± 15 MHz and 2.5 kW has been developed to create the pro ess for indigenous development at any frequen y in the range of HF and VHF.
2. Design of broadband multi-element coupled lines for high power handling apability is suessfully completed.
3. A 200kW and 38 to 116MHz, ultra-wideband novel 3dB hybrid oupler is designed, developed, fabricated and tested for the desired performance.
4. Design and fabrication drawings of the 1.5MW ultra-wideband 3dB hybrid oupler for the ICRF heating in fusion grade rea tor is ompleted.

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International Parti ipation

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2. Design and development of a 3dB high power hybrid coupler.(Poster) Rana Pratap Y adav, Sunil Kumar and S. V. Kulkarni 6th ITER International School Ahmedabad, India, 02-06 Decmber 2012.
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4. Design aspect of the tandem 3dB hybrid oupler using matching stub for the rf heating of plasma in tokamak.(Talk) Rana Pratap Yadav, Sunil Kumar and S. V. Kulkarni 2nd ISRC, 21st October 2011, IPR Gandhinagar, India.
5. Design aspect of the tandem 3dB hybrid coupler for the ultra wide band frequen y range of (32-112)MHz. (Poster) Rana Pratap Y adav, Sunil Kumar and S. V. Kulkarni 1st ASRC, July , 3-4, 2012 , IPR Gandhinagar, India.
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Abstract

Polymer solar cells as well as dye sensitized solar cells are promising candidates for the flexible and low-cost photovoltaic devices. In the case of polymer solar cells the efficiency depends on several factors, such as, molar extinction coefficient of donor and acceptor materials, energy gap, energy level alignment between donor-acceptor phases, exciton dissociation, interface between donor and acceptor phases, extraction and collection of carriers and selectivity of hole/electron transport layers etc. For dye sensitized solar cells the major factors that govern the efficiency are molar extinction coefficient of dyes, energy gap, energy level alignment between dye and TiO_2

semiconductor, charge injection, charge recombination, electrolyte leakage and evaporation, catalytic activity of counter-electrodes etc. However, in both polymer and dye sensitized solar cells, recombination is a major factor that strongly influence the efficiency. In case of polymer solar cells, geminate and bimolecular recombinations are predominant, whereas in case of dye-sensitized solar cells recombinations at TiO_2-dye (recombination with the oxidized dye) interface, and TiO_2-electrolyte (recombination with the oxidized redox mediator) interface are significant. In both devices, presence of disorders at the interfaces causes trapping of charge carries, which enhances the charge recombination. Therefore, in order to enhance the efficiency it is essential to minimize the disorders in the devices, which can be done by optimizing the materials parameters (i.e. morphology, structure, interfaces etc). Therefore, this thesis aims at developing low-cost photovoltaic technologies involving polymer solar cells and dye-sensitized solar cells, and improve their efficiency/stability by optimization of various device parameters, selection of appropriate materials, device structures and understanding of processes etc.

In the case of polymer solar cells, various studies pertaining to bulk-heterojunction P3HT:PCBM, porphyrin/polyfullerene diffuse bilayer solar cells, and porphyrin-modified ZnO-NW/P3HT hybrid solar cells are presented. The devices characteristics of P3HT:PCBM bulk-heterojunction solar cells were found to depend upon annealing temperatures. Therefore, temperature dependent in-situ Raman spectroscopy along with optical microscope of P3HT:PCBM films were investigated to gain insight into the structural and morphological changes. Diffuse bilayer solar cells, were fabricated by simultaneous deposition of porphyrin and fullerene films on ITO substrates yielding moderate photo-responses. In hybrid solar cells, the modification of ZnO-NW surface with porphyrin yields better performance as compared to ZnO-NW/P3HT configuration.

In the case of dye-sensitized solar cells, the devices were fabricated using different photoanodes, electrolytes and counter-electrodes. Briefly, we show that a proper selection of an organic dye with ZnO photoanodes results in better performances compared to their ruthenium counterparts. In addition, the major recombination loss in TiO_2 photoanodes was restricted with an application of co-adsorbent (formic acid), which later used as an anchoring site for a co-sensitization of two dyes resulting in improved efficiencies. A gel polymer electrolyte was synthesized to prevent common leakage and evaporation problem of typical liquid based electrolytes. A novel free-standing polypyrrole films synthesized by interfacial polymerization were applied as substrate-free, TCO-free counter-electrodes for cost effective DSSC.

An efficiency of 3.2% was obtained in P3HT:PCBM bulk-heterojunction solar cells and 5.2% in dye-sensitized solar cells. Finally, a correlation has been established between measured photovoltaic parameters and evaluated device parameters. In particular, the ideality factor in both the cases decreases as the efficiency of the device increases, indicating that recombination present at various interfaces are greatly reduced.

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Abstract

The studies presented in this thesis are concerned with VUV spectroscopic investigations of electronic states of molecules in gas phase in 35,000–95,240 cm^{-1} (4.3–11.8 eV) using synchrotron radiation. Comprehensive investigations of the VUV absorption spectra of the dihalomethanes CH_2X_2 (X= Cl, Br, I) and their isotopologues CD_2X_2 are presented. Most of the features are assigned to Rydberg transitions converging to the first four ionization potentials of the dihalomethanes based on quantum defect analysis. The spectra are analyzed in the light of TDDFT calculations to obtain better understanding of the Rydberg/valence nature of the excitations and their interactions. Observed vibronic features are assigned based on computations of equilibrium geometries and vibrational frequencies in the neutral and cationic ground states. Low lying electronic transitions as well as anomalously high intensities observed in the region of the Rydberg series are attributed to valence transitions with high oscillator strengths.

VUV photoabsorption studies and associated UV/VUV photodissociation processes of dimethyl sulphoxide (DMSO) and its counterpart dimethyl sulphoxide-d_6 (DMSO-d_6) are presented. The observed absorption spectral features are analyzed and interpreted in terms of valence transitions and Rydberg series converging to the first three ionization potentials of DMSO. Rydberg series are extended to higher members as compared to earlier works. Analysis is aided by quantum chemical calculations. Vibronic structures observed are re-examined by comparison of the spectra of the two isotopologues. In higher resolution studies completely different spectral features of DMSO are observed. Most of these features are identified and assigned to electronic or vibronic transitions of the SO radical. It is concluded that SO is prominently produced in the UV-VUV photodissociation of DMSO brought about by the incident intense broadband radiation in the experimental configuration used.

VUV studies of nitrous oxide (N_2O) in 71,800–95,240 cm^{-1} (8.9–11.8 eV) are presented. The analysis of the spectrum is carried out with the help of quantum chemical calculations of vertical excited state energies. The spectral features are assigned to a few valence transitions and several Rydberg series converging to the two spin orbit components of the ground state of N_2O^+. The comprehensive experimental data supported by extensive theoretical calculations have resulted in unambiguous assignments and clarification of discrepancies in earlier work.

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Abstract

Metal oxide semiconductors, both n-type (SnO_2, WO_3, ZnO etc) and p-type (Cr_2O3, CuO etc) are well established class of functional materials for chemiresistive gas sensors. Metal oxides are intrinsically insulators but presence of natural defects during their synthesis give rise to significant conductivity (n-type or p-type depending upon the nature of defect). This makes metal-oxides suitable for gas sensing, as their electrical resistivity (or conductivity) change upon interaction with analyte gas molecules. The chemiresistive sensors have extensively been investigated in different forms such as bulk pellets, thick films, thin films and nanostructures. Thin films and nanostructures offer various advantages: (i) larger surface area to volume ratio, implying more active sites for oxygen adsorption, (ii) Debye length comparable to the grain size or structure size which enhances the sensitivity; and (iii) small size of the sensors implying low power consumption if the sensor is operated at higher temperatures. Nanostructure based sensors have additional advantages in terms of possibility of high integration densities, ease of incorporation into microelectronic devices and superior stability owing to high crystallinity.

A major issue with pure metal-oxides sensors is the lack of specificity i.e. same sensor detects many gases. The use of additives has been widely employed for improving the selectivity. From the perspective of India, selective H_2S sensors are needed for Heavy water plants to monitor its concentration in environment (in case of any leakage). In literature, several additives have been employed to make metal-oxides sensors selective to H_2S. However the mechanisms of enhancement of the H_2S specificity by additives are not fully understood. Therefore, this thesis aims at understanding the gas-sensing mechanisms in metal-oxides chemiresistive sensors with suitable additives that make them selective to H_2S gas. We have synthesized p-type (CuO) as well as n-type (ZnO, WO_3, SnO_2) metal-oxides thin films and nanostructures for H_2S sensors. In addition, these thin films and nanostructures are tailored using suitable additives so as to realize highly specific either p-n junctions (CuO:ZnO, CuO:WO3, Fe_3O_4:SnO_2) or Schottky barriers (Au:ZnO, Au:WO_3) which enhances the specificity for H_2S. The gas sensing mechanisms were investigated using various techniques like X-ray photoelectron spectroscopy, impedance spectroscopy, Kelvin probe, photoluminescence, UV-Vis spectroscopy, X ray diffraction.

We have fabricated H_2S chemiresistive sensors based on n-type, p-type, p-n junction type and Schottky barrier type, and investigated their sensing mechanisms. Based on the results of this thesis work, H_2S sensors suitable for different concentration ranges are as follows:

- Sub ppm H_2S sensors: The chemiresistive sensor based on CuO thin films and Au:WO_3 Schottky barrier has the lowest detection limit of 100 and 50 ppb respectively.
- 1-50 ppm H_2S sensors: The chemiresistive sensors based on CuO:ZnO, CuO:WO_3 and Fe_3O_4:SnO_2 p-n junctions, sputtered SnO_2 thin films and Au:ZnO Schottky barriers were able to detect H_2S in the intermediate range with full recovery. Au: ZnO Schottky barrier based chemiresistive sensors could sense H_2S at room temperature. Also Fe_3O_4:SnO_2 p-n junctions type sensors showed the fastest response kinetics of 90 and 98 s respectively.

>50 ppm H_2S sensors: The chemiresistive sensors based on CuO islolated nanowires showed full recovery at high concentrations of H_2S but stability was a major issue due to poor electrical contacts to the individual nanowires.

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Abstract

The work in this thesis is based on the design of a high intensity proton drift tube linac for LEHIPA at BARC and the RF characterization of a prototype.

Detailed design of a 3-20 MeV drift tube linac has been done. The cavity geometry optimization aim is to maximize the effective shunt impedance while keeping enough space inside the drift tubes for focusing quadrupoles and cooling water channel. The frequency analysis with tuners, vacuum ports and RF ports were done. Postcouplers have been designed to achieve field stabilization. The beam dynamics design aim is to have 100 % transmission and minimum emittance growth. The zero current phase advance has been kept below 90° in order to avoid space charge induced beam instabilities. The aperture to rms beam size ratio of 8 has been maintained everywhere in the linac. With these criteria, detailed beam dynamics through the DTL has been done. Three focusing schemes have been studied and based on these studies; the FFDD

focusing lattice has been chosen. The effect of space charge on the beam dynamics has also been studied. From these studies, it is concluded that the space charge effects are not significant at around 10 mA but increases at higher currents. If the tune depression is close to or goes below 0.4 even for a few periods, there is significant distortion in phase space and a consequent increase in emittance. For the designed DTL at 30 mA, space charge effects are observable and lead to emittance growth. The presence of errors in the real linac may exacerbate the situation and one may expect higher emittance growth and even beam loss. The effect of beam alignment errors, quadrupole alignment and gradient errors and RF errors has been analysed, based on which the tolerances on these parameters have been obtained. The effect of combined errors has also been studied.

The formation and evolution of beam halos in the DTL has been studied. It is seen that a perfectly matched beam shows a halo in the longitudinal plane. Halos due to beam mismatch were studied. The particle-core model is used to find the mismatch required to excite the three fundamental modes of the beam envelope; the quadrupole mode, the fast mode and the slow mode. These modes were excited by giving suitable mismatch in the simulations and the evolution of the envelope oscillations and build up of halo along the length of the DTL was tracked. These studies were done with uniform and Gaussian input distributions. With uniform distribution, the beam oscillations persist with nearly unchanged amplitudes throughout the DTL. On the other hand, for a Gaussian distribution, the amplitudes get damped as the beam travels through the DTL. This is because the free energy available with the Gaussian distribution, leads to faster emittance growth. The particle redistribution at the end of the DTL has been obtained. These distributions show the formation of beam halos. The maximum halo extent was 6.6 times the rms beam size for 30 % fast mode excitation. However, there is no beam loss, since the aperture is 8 times the rms beam size. Based on definition of Allen and Wangler, the halo parameter has been calculated for the three eigen modes. The halo definition proposed by Nghiem has been used to determine the percentage of halo size and the percentage of halo particles. Two cases of general mismatch have also been analysed. The effect of varying beam currents on halo has also been studied and it is clear that halo grows with beam current. Longitudinal halos are formed even for a perfectly matched beam at currents of 20 mA and above. Transverse halos arise in the presence of mismatch and increase with increasing degrees of mismatch.

In order to validate the electromagnetic design of the DTL, a 1.2 m long prototype consisting of the first 17 cells of the first tank of the DTL, was fabricated. The prototype had three tuners, one vacuum port and two rf ports. RF measurements were performed on the prototype. The measured frequency agreed well with the simulations. Bead pull measurements were done to characterize the electric field along the axis of the DTL. A field uniformity of ± 2 % was achieved with the help of tuners. The value of RT /Q was also estimated from the measurement and agreed with the simulated value.

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Title	:	Ultrasonic Nondestructive Evaluation of Type 316 Austenitic Stainless Steel by Time-Frequency Analysis Methods

Abstract

The primary aim of the ultrasonic non-destructive investigations carried out in this thesis was to develop various time-frequency based signal processing methodologies to analyse ultrasonic signals for determination of grain size and detection of defects in type 316 austenitic stainless steel, with enhanced sensitivity. The time-frequency (TF) based signal processing techniques including short time Fourier transform (STFT), continuous wavelet transform (CWT) and ensemble empirical mode decomposition (EEMD) have been used. Specific software has been developed in LabVIEW and Matlab programming systems for accurate estimation of ultrasonic spectral parameters.

The time-frequency based approaches used in the study provided better understanding of frequency dependent attenuation in highly scattering austenitic stainless steel. The limits on the range of grain size imposed by conventional ultrasonic methods forits evaluation could also be overcome by the STFT and CWT based approaches. The shift in the peak frequency with propagation distance observed by the experimental results and mathematical model, paved the path for development of a single wavelet scale based CWT approach. This approach was used successfully for detection and imaging of defects at various depths in thick coarse grain austenitic stainless steel specimens. The novel adaptive methodology developed by employing signal minimisation algorithm on selected intrinsic mode functions(IMFs)obtained by EEMD showed better than 15 dB enhancement in the signal to noise ratio (SNR) of the ultrasonic signals. The EEMD with minimisation has been successfully used as a signal analysis approach for automatic defection of defects with improved sensitivity in coarse grain austenitic stainless steel.

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Title	:	On Verifying Proofs in Constant Depth, and Polynomial Identity Testing

Abstract

The thesis is divided into two main parts. The first part deals with proof systems that can be computed by boolean circuit families that characterize the complexity class NC^0 (bounded fanin, constant depth), which is one of the weakest complexity classes. A proof system for a language L is a function f : $\{0,1\}^m$ ^ $\{0,1\}^n$ such that Range(f) = L. We initiate a study of NC^0 computable proof systems with an overarching goal of showing that such proof systems cannot capture the language Taut. We begin by studying NC^0 proof systems in the context of regular languages. We give sufficient conditions for a regular language to have a proof system computable in NC^0. On the other hand, we show a regular language that does not have a proof system computable in NC^0. By generalizing techniques used in constructing proof systems for regular languages, we construct NC^0 proof systems for languages from various complexity classes ranging from $NC^!$-complete to P-complete. It remains open to characterize the regular languages that indeed have proof systems that are computable in NC^0. In the context of Taut, we study 2TAUT and show a reduction from 2TAUT to the language associated with directed connectivity in terms of proof systems. We show that the set of all undirected graphs that have a path between two fixed vertices s and t has an NC^0 proof system. Our study shows that there is no correlation between the languages that can be generated using these proof systems and the computational complexity of their associated membership problem.

In the second part of the thesis, we study the problem of testing if a given arithmetic circuit is computing the identically zero polynomial (PIT) and give efficient algorithms for certain special cases. We also determine the complexity of other natural problems that arise in the context of arithmetic circuits. We give a non-blackbox multilinearity and identity test for read-thrice formulas. Our algorithms look at circuit structure and use purely combinatorial ideas. We then give efficient algorithms for PIT on polynomials of the form $fif_2f_3 \bullet \bullet \bullet f_m + gig_2 \bullet \bullet \bullet g_s$ where fis and g,s are presented as ROFs. We show a hardness of representation for the elementary symmetric polynomial against read-once formulas with the added restriction that every leaf has to look like ax where a is a field element and x is a variable. Finally, we study some natural problems in the context of arithmetic circuits. These include counting number of monomials, and checking if a given monomial has non-zero coefficient in the polynomial computed by a given arithmetic circuit. We observe that even for monotone (no negative constants) read-twice formulas, counting the number of monomials is #P-hard. We also show that checking if the coefficient of a monomial is zero in a polynomial computed by a read-once formula is in logspace.

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Title	:	Silver Endotaxial Nanostructures in Si and their SERS Applications

Abstract

Endotaxy is growth of coherent structures inside a single crystalline substrate unlike the epitaxy, which is basically growth on crystalline layers. Epitaxy is well studied while endotaxy is not explored barring a few reports. Growing coherent noble metal nanostructures would help in finding out new applications where the combined advantages of noble metal nanostructures and semiconductors could effectively be coupled. This thesis reports a novel way of growing silver endotaxial structures in silicon single crystalline substrate of various orientations, characterize the structures with many complimentary experimental methods. The thesis reports on the applications of endotaxial silver nanostructures as robust and re-usable Surface enhanced Raman spectroscopy substrates to detect organic analyte molecules like crystal violet(CV), Rhodamine 6G (R6G) and bio-molecules like Creatinine.

In this thesis, novel methods have developed in facilitating the growth of endotaxial structures. The role of interfacial layers such as SiO_x and/or GeO_x has been studied extensively. The GeOx layer have deposited on various orientations of silicon substrates such as (100), (110) and (111). Two commonly known methods have been used, such as, physical vapor deposition (PVD) and chemical vapor deposition (CVD) to provide Ag film and Ag vapors, respectively. In case of PVD, a thin layer of Ag deposition at room temperature has been done using high vacuum coating unit and then annealing of system (Ag/GeOx/SiOx/Si) at various temperatures (maximum up to 900 C) has been carried out at various ambient conditions. For the CVD growth mode, GeOx/SiOx/Si system has been kept in a furnace along with a Ag wire. The high temperature in the furnace provide source for Ag vapors and for the reaction between GeOx and native oxide; this reaction process also depends on the partial pressure of residual or intended gas molecules (such as Oxygen and Argon or low vacuum conditions). Characterization of these annealed samples was done using transmission electron microscopy (TEM), scanning transmission electrons microscopy (STEM), scanning electron microscopy (SEM), synchrotron X-ray diffraction and Rutherford backscattering spectrometry experimental methods. Most of the study was done on Si(100) orientation including the 3-dimensional shape study of these nanostructures using STEM based electron tomography. Role of GeO_x presence on the silicon substrate as well as position of GeOx was also studied for Si(100) orientation.

Effect of annealing ambience on these endotaxial structures formation was also studied by considering GeO_x/Si(100) substrates. Substrates were annealed in different ambient conditions such as oxygen flow, low vacuum, ultra-high vacuum, argon flow and as well as normal-air ambience. Variation in shapes, size and dielectric media around these nanostructures was also discussed. In-situ and real time synchrotron x- ray diffraction and x-ray reflectivity measurements just above the Ge absorption edge were carried during the annealing of these samples to understand role of surface and inter-facial energies of these nanostructures formation. In this case, all the three substrate orientations were studied. Endotaxial structures grown using CVD method showed that temperature of the furnace and heating time duration plays an important and one can control the size, shape and type of structures.

As grown nanostructures by both CVD and PVD methods were covered with GeO_x and SiO_x layers. These oxide layers were removed using chemical etching to use the nanostructures as SERS substrates to detect analyte molecules like CV and R6G. These analyte molecules were detected with appreciable enhancement factors. Different shapes with different coverage were used to

understand the effect of shape and coverage on the enhancement factors was studied. Detection of Creatinine was also done with these endotaxial nanostructures.

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Title	:	Study of Group-IVB Metal Oxides in Bulk and Lower Dimension using Perturbed g-g Angular Correlation Technique

Abstract

The present thesis describes the development of a fast-slow coincidence setup for the Time Differential Perturbed Angular Correlation (TDPAC) measurements based on $LaBr_3$( ) detectors and then, hyperfine study of different physico-chemical phenomena related to group-IVB metal oxides using the above TDPAC spectrometer. The thesis envisages the sensitivity of the present nuclear hyperfine technique TDPAC in order to study chemical matrices in atomic level.

The latest available $LaBr_3$(Ce) scintillation detectors coupled to a fast PM Tube have been used in the above circuit. After coupling the detector-assembly to the coincidence circuit, the characteristics of the detector system has also been studied in order to optimize the best operational condition for the present measurements. This setup was used for the subsequent TDPAC measurements in order to study the different chemical phenomena. The TDPAC study of the pure Ti, Zr and Hf-oxides in bulk has been carried out and it has been extended to nano dimension in order to study the phase transition in pure TiO_2 nanoparticles as well as Ag@TiO_2 core-shell nanoparticles. The study of the doped systems, viz., Mn and Zr-doped TiO_2 system has also been carried out to investigate the metal-metal interaction in atomic scale. The study includes the thermal behaviour of HfO2 in its fiber and thin film forms. In some cases, the experimental results have been corroborated by the theoretical calculations of EFG at ^{181}Ta site using Wien2k code. The nuclear probe used in the present study, i.e., ^{181}Hf/^{181}Ta, falls in the same group and hence, has got the maximum probability to replace the lattice site in any of these three oxides prepared by a soft chemical coprecipitation method along with the probe. Another aspect of TDPAC, viz., the effect of radioactive decay process feeding the γ-γ cascade has also been studied with ^{111}In/^{111}Cd probe in case of pure oxides. In some cases, the present work has confirmed the pre-existing TDPAC data and in some cases, it has delivered several new data in the field of TDPAC.

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Title	:	Physics of Virtual Cathode Devices and Development and Validation of their Simulations

Abstract

In this thesis, we have first described the development of 2-D and 3-D Partiele- in-Cell codes used for simulating vircators. We also describe the methods used to validate these codes against published e xperimental and theoretical results. These codes have been parallelized to make efficient use of High Performance Computing facilities. The major findings of simulation studies using these codes are summarized below.

Firstly, 2-D, relativistic, electromagnetic PIC simulations show that with a copper foil anode, the output frequency of the vircator is strongly dependent upon the variation of foil transparency with electron energy. Using an average transparency for all electron energies yields results that are markedly different from those obtained using the actual variation. However, the output power shows only mild sensitivity. Hence the transparency has been calculated using a Monte Carlo code for electron transport through solids. Using the full energy-dependent form of the transparency, we get fairly good agreement with published experimental results.

Secondly, we report on the observation of a secondary virtual cathode. During periods of significant microwave emission, we observe the formation of a secondary, smaller, virtual cathode at some distance from the main virtual cathode. For a given vircator geometry, this appears only during low-voltage operation. The electron density in this secondary structure tends to increase with the microwave emission. We have also provided a physical explanation for the creation of this secondary structure and for its appearance only during low voltage operation. We find that electron trajectories in the vircator can be divided into four broad categories, based on their shapes and also on the temporal variation of electron kinetic energy. Three of these trajectories are those reported earlier by Alyokhin, while the fourth appears to be a new one. The fourth type is linked to the appearance of the secondary virtual cathode, and hence becomes significant only at times of significant power emission.

Thirdly, we have examined foil erosion due to ablation by the incident electron load, the expansion of the resulting plasma and A-K gap closure. We find that foil damage is generally higher near the axis. At all radial positions, there is little damage in the early stages, followed by a

period of rapid erosion, followed in turn by low damage rates, A physical explanation has been given for these trends. As a result of gap closure due to plasma formation from the foil, the output microwave power initially increases, reaches a near "flat-top" and then decreases steadily. For the parameters studied here, the output reaches a minimum around 230 ns. This is consistent with a typical plasma expansion velocity of ~2 cm/ps reported in the literature. We also find a significant variation in the dominant output frequency, from 6,3 to 7,6 GHz, This variation is small as long as the plasma density is small, up to 40 ns. As the AK gap starts filling with plasma, there is a steady increase in this frequency,

A detailed study, taking into account the effect of foil ablation for different foil thicknesses, shows that device performance is a complex function of foil thickness. For small thicknesses in the range 5-15 pm, for the parameters considered here, the peak microwave power emission tends to increase with increasing foil thickness. At thicknesses higher than 15 pm, the trend reverses, with a sharp reduction in power upto 60 pm. This is followed by a flat-top region extending upto 120 pm, followed by a second monotieally decreasing region. The trend in the low-thickness region has been explained in terms of foil damage, while the trend at higher thicknesses has been explained in terms of the time-averaged electron density in the virtual cathode 'cloud'. It is also observed that the dominant frequency of microwave emission decreases monotonieallv with increasing foil thickness. This is a result of systematic reduction in the peak density in the cloud. Another important finding is that under certain conditions, there is a periodic 'collapse' in the peak density of the electron cloud - this means that even though the peak density rises with increasing foil thickness, the time-averaged density, which determines the microwave power output, exhibits more complex behaviour.

Fourthly, for the first time, we have numerically examined the performance of a megawatt-nanosee class vircator operating in the Terahertz (THz) range. This work is a first step towards addressing the possibilities of short-pulse, high-power THz radiation from vireators, 2-D PIC simulations show that it is possible to operate vireators in the THz regime at a reasonably high power level of 0,4 MW, The pulse duration would be a few hundreds of picoseconds, and the dominant frequency is ~1 THz with a FWHM of ~ 8%, The small dimensions of such a device, and the required precision, would be experimentally challenging.

Finally, 3-D PIC simulations have been performed to examine the effect of non-axisymmetrv on vircator operation. Sample three-diimensional simulations, assuming one particular kind of anode misalignment, show a burn pattern as well as angular distribution of diode signal which exhibits large asymmetry. It also leads to generation of non-axisvmmetrie modes which are missing in axisvmmetrie systems. We further find that vireators operating in the THz regime are more sensitive to misalignments than GHz-class devices. Just one degree of misalignment in the foil can substantially change the output frequency as well as power level. Also, non-axisvmmetrie modes become stronger than axisvmmetrie modes for even small asymmetries in foil alignment. Hence precision fabrication would be an important consideration for THz-elass vireators.

Publications

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Title	:	Some Applications of Hard Thermal Loop Perturbation Theory in Quark Gluon Plasma

Abstract

It is now well-known that colored quarks and gluons are confined within color singlet hadronic bound states by strong interactions. As hadronic matter is heated and/or compressed hadrons occupy more and more of the available space within nucleus. Eventually they start to overlap and quarks and gluons confined initially begin to percolate between hadrons thus being liberated. Under this conditions quarks and gluons no longer remain confined within hadrons and a new state of matter known as Quark Gluon Plasma (QGP) is produced . The computation of Equation of State (EoS) is important as it is an important input to study the expansion dynamics of the hot and dense fireball produced in heavy-ion-collisions. The currently most reliable method for determining the EoS is lattice QCD. At this point in time lattice calculations can be performed at arbitrary temperature, however, they are restricted to relatively small chemical potentials. Alternatively, perturbative QCD (pQCD) can be applied at high temperature and/or chemical potentials where the strong coupling is small in magnitude; however, one does not know a priori how large the temperature should be for this method to result in a good approximation to reality. Unfortunately, in pQCD the resulting weak-coupling expansions are poorly convergent unless the coupling constant is tiny. Therefore, a straightforward perturbative expansion in

powers of running coupling for QCD does not seem to be of any quantitative use at the temperatures relevant for heavy-ion collisions. The source of the poor convergence comes due to the contributions from soft momenta, p ~ gT . This suggests that one needs a reorganization of finite-temperature and finite density perturbation theory that treats the soft sector more carefully. The hard-thermal- loop perturbation theory (HTLpt) is one of such reorganized perturbation theory at finite temperature and chemical potentials.

The HTLpt is a state-of-the-art resummed perturbation theory with a given mass prescription that reorganizes the usual perturbation theory at finite temperature/density. In HTL approximation the loop expansion and coupling expansion are not symmetrical. At each order in HTLpt the result is an infinite series in g, the strong coupling. Using the mass expansion one keeps terms through order g^5 (if one uses only LO mass prescription) all loop-orders of HTL perturbation theory in order to make the calculation tractable. In my doctoral tenure I have systematically computed various thermodynamic quantities viz. pressure, various order of quark number susceptibility, trace anomaly, speed of sound, entropy density etc. of hot and dense QCD matter within one loop (LO), two loop (NLO) and three loop (NNLO) HTL perturbation theory at finite temperature and chemical potential. For NNLO calculation we have used the two-loop perturbative mass prescription, the effective order of g becomes higher than g^5. The NNLO results are complete in g^5, gauge invariant and completely analytic that does not require any free fit parameter beside renormalization scale. The various quantities agree very well with lattice QCD results within error bars at the temperature down to 250 MeV.

As the dilepton rate is a good probe to study the deconfined state of matter, I have also analyzed the dilepton rates using HTL perturbation theory with various non-perturbative results obtained using Gluon condensate in the quark propagator, rho-meson-quark interaction in an effective model and lattice QCD. The results are contrasted with in-medium Hadron gas rate. Based on this, a more realistic way of the quark-hadron duality hypothesis is advocated than it was done in the literature.

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Title	:	A Study of Evolution of Microstructure Through Modeling and its Effect on Oxidation Behavior of Zr Based Alloys

Abstract

Zirconium based alloys are the workhorse materials for nuclear industry due to their excellent performance in reactor environment viz. low neutron absorption cross section, low neutron activation cross-section for induced activity, along with excellent corrosion resistance and superior dimensional stability. Current scenario demands nuclear power plants to operate under rigorous safety criteria. However, to be economically viable, it should operate at a higher temperature with modified environments such as the coolant with partial boiling to achieve high burn up and/or longer residence time of fuel. This has necessitated the development of advanced materials for fuel tube as well as pressure tube for third generation advanced nuclear reactors. The development of material for advanced nuclear reactor involves either optimizing the existing compositions or modifying the fabrication route leading to improved microstructure for final products or addition of new alloying elements.

To improve the mechanistic understanding of microstructural evolution in Zr base alloy and to predict the microstructure during diffusional phase transformation at various temperatures, phase field model has been developed for Zr-Nb series alloys during the course of this study using Gibbs free energy functional and diffusional mobility.

In multi-component Zr-Sn-Fe-Cr system, effect of size, distribution and micro- chemistry of second phase precipitates as well as the addition of Sn in Zr-Sn-Fe-Cr alloy and Fe in Zr-Nb-Fe system, on oxidation and hydrogen-pick up behaviour of the alloys have been studied. The oxidation experiments were carried out in steam at 415° C and 10 MPa pressure. The base metal microstructures were characterized systematically using scanning electron microscope (SEM), transmission electron microscope - energy dispersive spectrometry (TEM-EDS), small angle neutron scattering (SANS) after accelerated autoclaving. Oxide formed in each case at 415° C as well as in a few samples at 500° C autoclaving were examined through SEM, X-ray photo electron spectroscopy (XPS) and grazing angle incidence X-ray diffraction (GIXRD) technique. On few selected samples cross sectional TEM was carried out for detailed investigations. To assess the feasibility of simulation of in-reactor damage of oxide by ion irradiation, the behaviour of the oxide in Zr- 2.5Nb-Fe and Zr-Sn-Fe-Cr alloys was studied using the GIXRD technique, after irradiation by heavy ions and protons. The results were compared with the inpile oxide formed in fuel tube material during exposure in the temperature range of 260 - 263° C for 13 months in PHWR up to 7670 MWd/t burn up. GIXRD which is a nondestructive technique provides immense help in studying the distribution of phases in the oxide along the thickness direction without altering the stress pattern.

The detailed experimental and modeling studies of Zr base alloys performed during this period provide a comprehensive understanding of the evolution of microstructure specially Widmanstatten and allotriomorphic a during diffusional phase transformation in Zr-Nb base alloys. This thesis further discusses the effects of microstructure mainly second phase or precipitates size and distribution and the effects of alloying elements (Sn in Zr-Sn-Fe-Cr alloy, Fe in Zr-2.5Nb alloy) on oxidation and hydrogen pick up behaviour of the alloys. Finally the study improves in-depth understanding of irradiation induced phase transformation in oxide and distribution of phases in the oxide through thickness direction formed in the actual fuel tube during exposure in pressurized heavy water reactor (PHWR) and assesses the feasibility of simulation of the in reactor damage of oxide by ion irradiation.

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Abstract

A radiopharmaceutical is a radionuclide incorporating pharmaceutical preparation administered in vivo for clinical purposes, bearing adequate purity and pharmaceutical safety suitable for humans or animals. Over several decades, radiopharmaceuticals have been developed to non-invasively diagnose or treat a myriad of diseases, and cancer is one of the major areas for current research in this field. This thesis deals with development of novel cancer-related radiopharmaceuticals in two major areas: a) Sentinel lymph node (SLN) detection b) Hepatocellular carcinoma (HCC) therapy.

SLN detection is important for staging and prognosis of cancers of several origins. SLN radiotracers are typically nanoparticles that are phagocytized by lymph node macrophages, thereby retaining the radioactivity in the node. This is used to detect the SLN by suitable means. Here, different nanoparticles were developed using poly-lactide (co-glycolide) [PLGA] copolymer: a) PLGA b) Mebrofenin-loaded PLGA c) Diethylenetriaminepentaacetate (DTPA) conjugated PLGA. They were physico-chemically characterized, labeled with technetium-99m (^{99m}Tc), and tested in Wistar Rat model. Animal model studies showed DTPA-conjugated PLGA to have the best properties with regard to ^{99m}Tc-labeling and characteristics of uptake and retention in the SLN in animal model.
Dextran-Mannose radiotracers, expected to bind with mannose receptors of lymph node macrophages, were developed to overcome limitations of conventional nanoparticle SLN tracers. Two classes of derivatives were biologically evaluated: a) Dextran-Cysteine-Mannose (DCM20) b) Dextran-Pyrazolyl-Mannose (DAPM4 and DAPM8) These were tested in vitro in RAW 264.7 cells where they showed differing affinities. However in vivo studies, showed fairly similar SLN uptake and retention properties, with DCM20 having an edge in clearance from the site of injection.

For radio-embolic treatment of HCC two yttrium-90 (^{90}Y) strategies were developed: a) ^{90}Y-oxine in lipiodol b) ^{90}Y-Biorex 70 microspheres. The ^{90}Y-labeling characteristics were thoroughly studied - both showed good labeling yield and the microspheres showed excellent stability of ^{90}Y-label. Animal model of HCC was developed in Sprague-Dawley rat with N1S1 rat HCC cell line. The preparations were tested in the HCC model. At 7-days post-injection, while ^{90}Y-oxine in lipiodol showed leakage from the liver and activity in the bone, ^{90}Y-Biorex 70 microspheres were stably retained and also showed noticeable therapeutic effect as seen from histological and marker studies, thus showcasing potential for use in the clinic.

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Title	:	Charmonium Production and Suppression in Pb+Pb Collisions at $\sqrt{S_{NN}}$ = 2.76 TeV with CMS

Abstract

The primary goal of the study of ultra relativistic heavy-ion collisions is to create and characterize the Quark Gluon Plasma (QGP). In this thesis, we describe the production and suppression of prompt and non-prompt J/psi and the study on the relative suppression of J/psi and Psi(2S) using ratio of their yields. These measurements were performed with the data recorded by the Compact Muon Solenoid (CMS) experiment during the PbPb runs and during the pp runs, all at $Ös_{NN}$ = 2.76 TeV.

In the J/psi analysis, we measure the inclusive J/psi production produced in PbPb collisions at $Ös_{NN}$ = 2.76 TeV. Non-prompt J/psi from B hadron decays have been separated from prompt J/psi utilising the reconstructed decay vertex of the dimuon pair. Experimentally, the suppression is quantified by the nuclear modification factor, R_{AA}. A strong, centrality-dependent suppression has been observed for J/psi with p_T > 6.5 GeV/c. For non-prompt J/psi , the centrality dependence shows a slow increase of suppression with increasing centrality. This was the first detailed look at the b-quark energy loss dependence on centrality, p_T and rapidity.

In the charmonia double ratio measurement, we compared the ratio of prompt Psi(2S) over J/psi yields in PbPb and pp collisions in two kinematic bins, mid-rapidity (high p_T) and forward rapidity (from low p_T). Psi(2S) production is suppressed in PbPb collisions with respect to pp collisions, in both kinematic regions investigated. In comparison to J/psi production and in the most central PbPb collisions, Psi(2S) production is suppressed in the mid-rapidity bin, as expected in the sequential melting scenario, while it is enhanced in the forward rapidity bin. In the most central

collisions the double ratio becomes 2.31 ± 0.53(stat.) ± 0.37(syst.) ± 0.15 (pp) indicating that the Psi(2S) to J/psi yield ratio is enhanced in central PbPb collisions with respect to pp collisions.

This thesis includes a phenomenological study on quarkonium suppression due to color screening based on a dynamical model which takes into account lifetime and size of QGP. Using the model we estimated the survival probability of quarkonia as a function of p_T and centrality. Also we obtained the R_{AA} and the double ratio by applying the feed-down corrections. We compared our model calculations with CMS quarkonia results from PbPb collisions at Ös$_{NN}$ = 2.76 TeV.

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Title : Evaluation of Self-Welding Susceptibility of Austenitic Stainless Steel (Alloy D9 and 316LN) in High Temperature Flowing Sodium

Abstract

In Prototype Fast Breeder Reactor (PFBR), the subassemblies are provided with a pad on the six faces of the subassemblies at the top where contact is established between adjacent subassemblies. Flowing sodium at 823 K through the core removes the oxide layers from the mating surfaces of the subassembly pads and metal to metal contact take place leading to self-welding. A study on self-welding susceptibility of alloy D9 (which is the material chosen for subassembly contact pad) was taken up and compared with 316LN (the structural material chosen for reactor construction) taken as reference material. Worldwide, investigators have carried out self-welding experiments on 304, 316 and 321 austenitic stainless steel. Literature survey revealed that no work has been reported on alloy D9 and 316LN. In this research work self-welding susceptibility of alloy D9 in annealed and 20% cold-worked condition have been evaluated in flowing sodium at 823 K for a contact stress range of 9.4 MPa to 24.5 MPa and for durations of 3, 4.5, 6 and 9 months. Similarly, self-welding susceptibility of 316LN was also studied in annealed and 20% cold-worked condition and compared with the results of D9.

In this experiment, a dedicated sodium facility was used. The specimens tested in the experiment were hollow cylindrical stacked one above the other under compression using Belleville spring to get the required contact stress. The mating surfaces of the specimens were polished and surface roughness was maintained below 0.5 µm. Specimen assembly is then put inside the test vessel of sodium facility. Initially the specimens contact surfaces are allowed to come in contact with pure sodium flow which removes the oxide layer from the mating surface. After 24 hours the specimens are compressed by Belleville springs. The sodium loop is operated for the specified period and sodium purity is maintained by cold trapping continuously. The contact load in the specimen is also maintained uniformly using the load cell till the end of the experiment. After the experiment, the sodium is drained and test vessel is cooled to room temperature. The specimens are taken out with sodium deposits. Cleaning of specimens was carried out with alcohol. The self-welded specimen pairs are separated by a set up to measure the shear force. The tested specimens were later analyzed for self-welding using self-welding coefficient, SEM, EDS, Macro and Micro hardness.

The results indicated that the self-welding tendency is more in annealed 316LN than in 20% cold-worked 316LN which is on the expected line. On the contrary, 20% cold-worked alloy D9 showed more self-welding tendency and the annealed alloy D9 showed no self-welding. On analysis it was found that dynamic recrystallisation favoured self-welding tendency in 20% cold-worked alloy D9 and there was no dynamic recrystallisation in annealed alloy D9. The carburisation of alloy D9 in sodium resulted in the formation of TiC precipitates at the grain boundary near the surface which accelerated the dynamic recrystallisation in 20% cold-worked alloy D9. Thus 20% cold-worked alloy D9 was found to be more susceptible for self-welding in flowing sodium. It was also determined that for PFBR conditions, self-welding will not occur in 20% cold-worked alloy D9 contact pads of the subassemblies during its operation.

Publications

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Abstract

The thesis concentrate on production and suppression of bb bound states, namely Y(1S), Y(2S) and Y(3S) which are measured in pp, pPb and PbPb collisions at LHC. This is the first time we are able to measure all three Y states separately with good statistics thanks to the large integrated luminosity and high-tech detectors available at LHC.

The measurement presented here use the PbPb and pp collision data recorded by the Compact Muon Solenoid (CMS) experiment at $^{Y}s_{NN}$ = 2.76 TeV . The Y states are identified through their dimuon decay. Muons are reconstructed by matching tracks in the muon detectors and silicon tracker. Only muons with a transverse momentum (pT) higher than 4 GeV/c and n < 2.4 are considered. A simultaneous fit to the pp and PbPb mass spectra gives the double ratio, |¼(2s¼3S)¾aS^{PbPb})' 0.31-0'19(stat) ± 0.03(syst). It was the first indication of relative suppression of excited Y states in PbPb collisions. To measure the absolute suppression of Y(nS) states, an update of these measurements is performed, utilizing the large PbPb data sample collected in by CMS in December 2011. Absolute suppressions of the individual Y states and their dependence on the collision centrality are studied. The results indicate a significant suppression of the Y(nS) states in heavy-ion collisions compared to pp collisions. The data support the hypothesis of increased suppression of loosely bound states. The suppressions are also observed to increase with collision centrality.

To constrain the cold nuclear matter effects, production of Y states is measured in pp and pPb collisions. Y(nS) are studied as a function of event activity estimated by mid rapidity charged-particle multiplicity and forward rapidity transverse energy. The Y yields normalized by their event average, Y(nS)/(Y(nS)>, rise with both measures of the event activity in pp and pPb. In both datasets, the ratios of the excited to the ground state, Y(nS)/Y(1S), decrease with the charged-particle multiplicity but does not show a definite trend when measured as a function of the transverse energy. The event-activity integrated double ratios, are also measured and found to be less than one but significantly above the PbPb double ratios. This observation indicate presence of additional final state effects in PbPb collisions.

This thesis consist of measurements as well as theoretical calculations. With the aim of background estimation in dimuon spectrum, we calculate open charm and bottom production and determine their contributions to the dimuon continuum in PbPb collisions at ySNN = 2.76 TeV with and without heavy quark energy loss. These rates are then compared with Drell-Yan and thermal dilepton production. The contributions of all these sources are obtained in kinematic regions relevant for the LHC detectors. It is found that dileptons from DD decays dominate over the entire mass range due to the large cc production cross section. To understand contribution of different mechanisms responsible for quarkonia suppression, we estimate the modification of quarkonia yields in the medium produced in PbPb collisions at LHC energy. A kinetic model is employed which incorporates quarkonia suppression inside QGP due to gluon dissociation, suppression due to hadronic comovers and regeneration from uncorrelated thermal charm quark pairs. The manifestations of these effects in different kinematic regions in the nuclear modification factors for both J/^ and Y has been demonstrated for PbPb collisions at $^{Y}s_{NN}$ = 2.76 TeV in comparison with the measurements.

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Abstract

My PhD work is concerned with various research activities in the frontier areas of chemical sciences involving introduction of new chemical concepts using density functional theory and predictions of the structure and properties of novel chemical systems in their ground and excited states through large scale computations based on first-principle computational methodologies.

In particular my work is mainly focused on two important aspects viz. theoretical designing new actinide selective ligands for lanthanide-actinide separation followed by experimental validation, and design of nanoscale carbon based adsorbent materials for radionuclide immobilization through large scale computations within the framework of density functional theory.

I have designed novel ligands for selective extraction of actinides from lanthanides, which is very important from the view point of nuclear waste management. In this field I have proposed a new concept, "Intra-ligand Synergism", and demonstrated that trivalent actinide can selectively bind with hard oxygen donor ligand in presence of soft donor ligand through designing new actinide selective ligand based on the derivatives of phenanthroline dicarboxylic acids. It is in sharp contrast to the conventional design methodology, where soft donors are generally used to achieve actinide selectivity. Experimental validation of this theoretical prediction has also been pursued through synthesis of the newly designed ligand followed by solvent extraction experiments. This work has opened up a new dimension in the field of separation science involving trivalent actinides and lanthanides and would have important implications in nuclear waste management.

Since, the selectivity of a particular ligand towards a particular metal ion can be rationalized in a better way through theoretical modeling studies, we have also theoretically investigated few well known actinide selective extractants to rationalize some of the experimentally observed trends.

Apart from designing novel actinide selective ligands, I have also predicted new highly stable actinide-lanthanide encapsulated metallofullerenes. Smaller fullerenes are of special interest due to the presence of high curvature and huge strain energy owing to the presence of adjacent pentagonal rings, which lead to clusters with unusual intra and inter -molecular bonding and electronic properties. The smaller fullerenes, which are formed during the production of stable fullerenes, are difficult to isolate because of their extremely high chemical reactivity. Thus, synthesis of smaller size fullerene has been a great challenge to experimentalists because of its high reactivity. I have proposed and demonstrated a novel scheme, through which smaller size fullerenes can be stabilized through encapsulation of an actinide or lanthanide metal atom/ion with certain number of valence electrons resulting into highly stable magic systems. High stability of these clusters have been rationalized through fulfillment of 26 and 32 valence electron principles.

These smaller size metallofullerenes can be extremely useful for their potential applications in nuclear medicine, as reported for larger metallofullerenes. Moreover, following this scheme it may be possible to entrap different actinides into carbon nanostructures, resulting into chemically stable radionuclide encapsulated bio-compatible fullerenes for various applications including safe management of nuclear wastes and designing cluster-assembled novel materials.

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Abstract

In this thesis, broadly three issues regarding black holes in loop quantum gravity(LQG), modeled as quantum isolated horizons, are discussed.

Firstly, the calculation of microcanonical entropy of black holes within the tenets of a modified paradigm within LQG framework. The physical consequences following from the calculations are discussed, with an emphasis on the fact that all the results and the relevant physics related to this modified paradigm are realizable from within the Chern- Simons description of the horizon degrees of freedom in the LQG framework, without having to incorporate any sort of semi-classical approximations gleaning out of LQG.

Secondly, the partition function for charged black hole horizons is derived using the structures and results of LQG description of black holes, without using any metric from the classical theory. Thermodynamic stability criteria for charged quantum black holes under Gaussian thermal fluctuations are derived in the form of differential inequalities, which are used as testing tools to examine the thermodynamic stability of charged black holes with known mass functions. For example, the stability criteria successfully explain the stability and instability of asymptotically flat and AdS Reissner-Nordstrom black holes.

Finally, the issue of energy spectrum of equilibrium black holes in LQG is discussed. A model Hamiltonian operator for the quantum isolated horizon is proposed. Demanding that the energy spectrum should consistently lead to the notion of classical energy arising from the first law of horizon mechanics, the unknown coefficients and parameters of the model are fixed, yielding the final form of the Hamiltonian operator.

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6. Abhishek Majhi - Energy Spectrum of equilibrium Black Holes, arXiv:1303.4832
7. Abhishek Majhi - An account on statistical mechanics and thermodynamics of quantum isolated horizons; arXiv:1312.0062

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Abstract

A superheated droplet detector (SDD) consists of a large number of droplets of a superheated liquid suspended in another immiscible liquid-like, soft gel medium or a firm polymer matrix. The basic principle of operation of SDD is similar to that of a bubble chamber : The superheated state being metastable, the passage of an energetic particle through a droplet can trigger a 'nucleation' event, whereby the energy deposited by the particle within the droplet can cause a phase transition of the metastable liquid phase to the vapour phase. If the energy deposited by the particle within a certain critical length is larger than a certain critical energy, the vapour bubble grows, eventually converting the whole liquid droplet into the vapour phase. The acoustic pulse generated in this process constitutes the signal of passage of the particle, which is recorded by acoustic sensors. This thesis presents a detailed study of the response of SDDs to various kinds of particles such as neutrons, alpha particles, gamma rays and heavy ions, with a view to a better understanding of the working principles of SDDs in general and towards developing effective procedures for discrimination of nucleation events due to various particles (neutrons, alphas, gamma rays, etc.) that are known to be responsible for the background events in experiments for direct detection of Weakly Interacting Massive Particle (WIMP) candidates of dark matter (DM) using SDDs. The thesis is divided into two parts: The main objectives of Part I are (i) to study the response of the SDD to heavy ions and, in particular, to study the dependence of the nucleation parameter (k) on the mass of the heavy ions with the help of GEANT3.21 simulation toolkit, and (ii) to study discrimination of neutron and gamma-ray induced nucleation events in SDDs with different active liquids by performing experiments. The present simulation provides an important observation that the nucleation parameter decreases with the increase in mass number of the heavy ion and the results of experiments clearly demonstrates for the first time the possibility of identification of and hence discrimination between neutron and gamma ray induced nucleation events by measuring the pulse height distribution in a mixed neutron-gamma radiation field. In Part II, certain issues pertaining to the application of SDDs in the direct detection of the WIMP candidates of DM by the PICASSO experiment (Project In CAnada to Search for Supersymmetric Objects) located at the SNOLAB underground facility in Sudbury, Ontario, Canada, are discussed. Specifically, results of investigations into the following aspects of the experiment are presented: (i) To understand the reason behind the two different threshold temperatures observed for a-induced events in the detector with the help of GEANT3.21 simulation, (ii) to study the role of the droplet size (of the active liquid) in the discrimination between a- and neutron induced nucleation events in the detector by performing experiments, and (iii) development of an analysis procedure to improve the resolution of discrimination between the a- and neutron (or nuclear recoil) induced events. From the results of the simulation, it is observed that the threshold temperature of alpha particles in the case of ^{241} Am spiked detector (for which the source of the a contamination is in the polymer matrix only) and the case of ^{226}Ra spiked detector (for which the a contamination is present both in the droplet as well as in the polymer matrix) is same, while the calculation of LET (Linear Energy Transfer) using SRIM2008 code explains that the higher LET of recoiling nuclei, Pb, of energy 146 keV coming from ^{226}Ra decay chain is responsible for the experimentally observed lower threshold temperature in case of ^{226}Ra spiked detector. These results of our simulation yield a proper understanding of the actual experimental results. We have performed experiments with superheated R-12 (CCl_2F_2, b. p. -29.8 °C) droplets dispersed in soft aquasonic gel matrix in presence of two neutron sources, namely, ^{241}Am-Be (3 Ci) and ^{252}Cf (3.2 pCi), and an a-source, ^{241} Am (30 particles s^{-1}) at the temperature of 33.5±0.5 °C to study a- and neutron induced nucleation events. The droplets of two different radius distributions (0-100 pm) are used. Instead of obtaining larger amplitude of pulses for alpha-particle induced events,

as previously observed by COUPP, PICASSO and SIMPLE experiments, both smaller and larger amplitude pulses are observed in our present experiments due to the different smaller droplet size distribution used in our experiment. We describe a new analysis method for obtaining a better a-neutron discrimination capability through the variable PVAR (which is a measure of the acoustic energy released during the bubble nucleation process) using PICASSO experimental data. It is observed that the value of this variable decreases with time which makes the PVAR distribution broader, thereby affecting the a-neutron discrimination ability. We have developed two correction methods to improve the resolution of PVAR distribution by controlling the effect of decrement of PVAR with time. This has resulted in significant improvement in the data analysis of the PICASSO experiment.

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   Nuclear Instruments and Methods in Physics Research A, 2013, 729, 182-187.

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Abstract

The fabrication of Zr-2.5Nb alloy pressure tubes is quite complex and involves hot deformation (forging and extrusion), heat treatment (quenching, annealing, autoclaving etc) and cold deformation (pilgering or drawing). In this research work, pressure tube material fabricated through two distinct routes which are generically known as cold work route and heat treated route, have been studied in detail. Hot extrusion stage is the most important fabrication step in the fabrication of the pressure tube manufacturing. In the present thesis FEM simulation of Hot extrusion process has been carried out.

The influence of process parameters associated with hot deformation, heat treatments and cold deformation have been systematically studied. In the cold deformation route nine distinct fabrication schedules were examined. These represented variations in (a) methodology of breaking cast structure (b) hot extrusion parameters (c) conditions of cold work and intermediate annealing. An optimized flow sheet could be developed on the basis of detailed characterization of the microstructure, texture and mechanical properties .The optimized process involved two stage forging followed by hot extrusion with higher extrusion ratio (12:1) and single stage of cold work without any intermediate annealing. This process resulted in desirable alpha morphology (1:10:80 aspect ratio) with a continuous fibrous beta morphology. The tube produced with this route had transverse basal texture component (f_t) above 0.6. Both this microstructure and texture are desirable for better creep resistance of the tube in reactor conditions. This route had also resulted in near elimination of end to end variation of the properties of the final tube.

On the basis of the present study on quenched microstructure, cold deformed and subsequent aged microstructure as a function of process parameters, optimized fabrication flowsheet to manufacture heat treated Zr-2.5 Nb alloy tube could be established. The optimized route included quenching (840^{o}C) followed by cold deformation by pilgering and aging at 540^{o}C for 24 Hrs. The resulting microstructure consisted of primary in conjunction with fine transformed lamellar having dispersed equilibrium globules inside it. The texture was also significantly different from that of the cold work route produced tube. However the mechanical properties were comparable.

FEM simulation of hot extrusion process has been carried to understand role of extrusion temperature, extrusion ratio, ram velocity and profile of die on the extrusion process for

obtaining desirable temperature, strain and strain rate distribution across the work piece. The model could be successfully validated against measured load data of the extrusion of actual pressure tube. The model could quantify the expected heterogeneity across thickness and length of the work piece as a function of various processing parameters.

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Title	:	Investigations on Pressure Induced B1-B10-B2 Phase Transitions in Binary Systems LAN, LIH and MGO

Abstract

High pressure research on materials has made significant advancement in past few decades. The advent of sophisticated static and dynamic high pressure generation techniques and diagnostic techniques has made it possible to examine the material behaviour in multimegabar pressure and high temperature regime. Several aspects of material behaviour examined in past include interesting structural phase transitions, metal to insulator and insulator to metal phase transitions, high pressure-high temperature equation of state, pressure effect on melting point, magnetic properties and vibrational properties. Apart from the experimental techniques a significant progress has been made in theoretical field also. The capability of calculating the total energy reliably and accurately for any kind of strain has made the modern ab-initio band structure methods an important tool not only to substantiate the experimental data but also to predict the material behaviour prior to the experimental investigations. In this direction, the present thesis investigates the high pressure behaviour of three binary compounds, namely LaN, LiH and MgO using the ab-initio electronic band structure methods. The theoretical work includes the analysis of structural stability, determination of 300 K isotherm, elastic constants and phonon spectra as a function of hydrostatic compression. For all these compounds existing in rocksalt structure (B1) at ambient conditions, the structural stability has been analyzed for three plausible structures namely B1, B10 (tetragonally distorted CsCl type structure) and B2 (CsCl type structure) as a function of hydrostatic compression. In LiH, structural stability analysis suggests that the B1 phase will transforms to B2 phase at ~327 GPa. Various equilibrium properties, e.g. the zero pressure equilibrium volume, bulk modulus and its pressure derivative, bulk sound velocity, the shock parameter, the Debye temperature and the Gruneisen parameter has been determined from the present calculations and compared with the available experimental data. The variation of elastic constants and elastic anisotropy as a function of pressure has been determined. Further, the phonon spectrum has been calculated as a function of pressure. The phonon spectrum calculated at zero pressure agrees reasonably with the experimentally measured data. The X- point phonon frequencies calculated at various pressures up to maximum of 120 GPa display a good agreement with the available experimental data. In MgO, the comparison of enthalpies of B1, B10 and B2 phases suggests the B1 to B2 structural transition at ~ 535 GPa. Further, the 0 K energy-volume relation in conjunction with thermal corrections has been utilized to derive the 300 K isotherm, isentrope and Hugoniot of this material. The theoretical investigations have been further extended to calculate the ideal strength of this material subjected to uniaxial compressive and expansive deformation along [001] crystallographic direction under two loading conditions namely “uniaxial stress condition” and “uniaxial strain conditions”, respectively. The ideal failure strengths for compression and expansion have been determined by examining the elastic stability conditions throughout the deformation path. The elastic stability condition suggested that for [001] uniaxial expansion, the MgO single crystal will fail due to vanishing of tensile modulus, whereas it will fail due to shear instability under uniaxial compressive loading. The ideal compressive strength and ideal tensile strength for compressive and tensile loading along [001] direction under uniaxial strain condition are determined to be —283 GPa and ~ 20 GPa, respectively; the same under uniaxial stress condition are calculated to be —115 GPa and ~11 GPa, respectively. In LaN, The theoretical calculations suggest the B1 to B10 (HP-LaN phase) transition at ~ 19 GPa as compared to the experimental value of 22.8 GPa. Further, we predict that the HP-LaN phase transforms to B2 phase at ~ 169 GPa. Band structure analysis suggests that the low symmetry HP-LaN phase could be stabilized at lower pressure due to symmetry breaking lowering of total energy. Apart from this theoretical work, the thesis also reports the experimental measurements of the tensile

fracture strength and yield strength of polycrystalline copper subjected to uniaxial loading at strain rates of ~ 10^4 /s. The yield strength and spall strength of 0.14 GPa and 1.32 GPa, measured at strain rates ~ 10^4 /s from free surface velocity history are higher than the 0.13 GPa and 0.22 GPa, respectively, measured in the quasi static loading condition. Further, the nanohardness and the Young's modulus determined from the nanoindentation method signify that the effect of shock treatment is increase the hardness and Young's modulus of this material.

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Title		Remote Field Eddy Current Based Approaches for High Sensitive Detection of Deffects in Ferromagnetic Steam Generator Tubes

Abstract

This thesis proposes different approaches for high sensitive detection of defects in ferromagnetic steam generator (SG) tubes using remote field eddy current (RFEC) nondestructive testing technique.

It proposes a new nonlinear finite element model to precisely identify the RFEC region (33 mm) for placing the receiver coil and to optimize the operating frequency (825 Hz) for enhanced detection of defects.

For reliable detection of defects in the bend regions of the SG tubes, continuous wavelet transform (CWT) based digital signal processing approach has been proposed. The wavelet transform based digital signal processing technique using the optimized Bior2.8 wavelet could reliably detect 0.23 mm (10% WT) deep grooves anywhere in the bend regions of the SG tube with SNR of 7 dB.

A first of its kind experimental investigation has been carried out, to study the influence of sodium deposits in the defect regions of the SG tube, on RFEC signals. An invariant parameter of the RFEC signals has been identified for detection and sizing of defects deeper than 0.23 mm (10% WT) in the presence of sodium deposits.
For detection of defects under Inconel support structures, a novel dual frequency mixing algorithm based on linear kernel transform (LKT) has been proposed. The performance of the mixing algorithm has been demonstrated on model predicted RFEC signals of grooves (depth 20% WT, 30% WT, and 40% WT) under support structures.

Capabilities of the approaches for detection of defects have been analyzed and future directions have been set towards high probability of detection of defects, anywhere in the SG tubes. The proposed approaches will enable reliable in-service inspection of SG tubes, ensuring structural integrity and safety of SGs.

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Title		Large scale behaviour of the freely cooling granular gas

Abstract

Freely cooling granular gas (FCGG) is a widely studied model to understand the role of dissipation in granular systems. In this model, particles are uniformly distributed in space initially. The particles move ballistically until they inelastic collisions. The system remains homogeneous for initial times and later evolves to inhomogeneous clustered regime due to dissipation. This inhomogeneous regime is poorly understood, and this thesis work is devoted to its understanding using numerical simulations.

In Chapter 4, we study FCGG in three dimensions. In the inhomogeneous regime, kinetic energy T(t) decreases with time t as a power-law $t^{\sim dT}$, where 6_T depends only on dimensionality D. Two

theoretical conjectures exist for the exponent 6_T. One is ballistic aggregation approach predicting $6^{BA} = 2D/(D + 2)$. The other is based on Burgers-like equation predicting $\$B^E = D/2$ when $2 < D < 4$. The exponents $\$B^A$ and $\$B^E$ coincide with each other in one and two dimensions, while they differ in three dimensions with $6^{BA} = 6/5$ and $6^{BE} = 3/2$. In numerical simulations, we found that that while $6_t \sim 6/5$ is as predicted by ballistic aggregation, the cluster statistics and velocity distribution differ from it. Thus, we conclude that FCGG fits to neither the ballistic aggregation or a Burgers equation description.

In Chapter 5, we study of the inhomogeneous regime of FCGG of rough particles in two dimensions. The translational kinetic energy and the rotational energy decay with time as power-laws $t^{\sim dT}$ and t^{-dR}. We numerically determine $6_T \sim 1$ and $6_R \sim 1.6$. Scaling arguments predict $6_T = 1$ and $6_R = 1$ for corresponding ballistic aggregation model, 6_R being different from that obtained for the rough granular gas. Simulations of ballistic aggregation are consistent with the scaling exponents. Mismatch of 6_K supports our earlier conclusion that ballistic aggregation is not a correct description of FCGG.

In Chapter 6, we study a special case of FCGG, called granular explosion model, where initially all particles are at rest except few in a localized space. We observe the clustering of all moving particles into a growing spherical shell, with vacant inside region. Radial momentum conservation argument predicts that radius of disturbance R(t) grows with time t as R(t) $_t$1/(D+1), which is confirmed in simulations. In a recent experiment [Physical Review Letters, 103, 224501(2009)], a monolayer of glass beads flowing down on an inclined plane was perturbed by dropping a steel ball. Our granular explosion model mimics the experimental system when one transforms to the center of mass coordinates. We show that our result $R(t) \sim t^{1/3}$ (in $D = 2$) fits very well to the experimental data except at large times. At long times the experimental data deviate from the $t^{1/3}$ behaviour. This, we argue is due to the experimental system becoming effectively three dimensional, and propose a simple model incorporating this effect. Our numerical data, obtained from simulations of this model captures the long time behavior.

In Chapter 7, we extended the study granular explosion model to viscoelastic particles, where coefficient of restitution r is velocity dependent. We observed the formation of band and the scaling results for radius of disturbance continue to hold for viscoelastic system.

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1. Shock propagation in granular flow subjected to an external impact S. N. Pathak, Z. Jabeen, P. Ray, and R. Rajesh Physical Review E 85, 061301 (2012)
2. Shock propagation in a visco-elastic granular gas S. N. Pathak, Z. Jabeen, R. Rajesh, and P. Ray AIP Conf. Proc. 1447, 193 (2012)
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Title		Differential calculus and Yang-Mills functional in Noncommutative Geometry

Abstract

This thesis is concerned with analyis of spectral triples as indicated in the last chapter of Connes' book. We study the Yang-Mills functional and the differential calculus of Connes'

The study of Yang-Mills functional in noncommutative geometry started with Connes-Rieffel when authors defined it on a C* -dynamical system. Later the spectral triple approach became more popular in noncommutative geometry and Connes defined the notion of Yang-Mills functional in this setting. There is a general recipe to produce a "spectral triple" from a C*-dynamical system but it does not tell whether the resulting object is a true spectral triple, but they are candidates, and one has to verify the relevant conditions on a case by case basis. However, for noncommutative torus and the quantum Heisenberg manifolds indeed one obtains a genuine spectral triple through this prescription. Then one encounters the natural question whether these two notions of Yang- Mills agree. A proposition in Connes' book suggesting the equivalence for the noncommutative 2-torus strengthens the point of showing equivalence. However, there is no proof available in his book. We show that for the noncommutative n-torus and the quantum Heisenberg manifolds both the approaches to Yang-Mills, the approach based on C*-dynamical systems and that on spectral triples, agree up to a positive constant.

The other part in this thesis deals with the study of Connes' differential calculus. Associated to every spectral triple there is a differential graded algebra, also called differential calculus, defined by Connes. This differential calculus is used to define the Yang-Mills functional based on spectral triples. Here we set ourselves with the task of understanding this concept. There is no general recipe to compute this calculus and instances of computations are very few available in the literature, only for some particular examples. The major difficulty in computation lies in identifying certain infinite dimensional spaces concretely. We compute this calculus for a large family of spectral triples. It should be noted that this is the first systematic computation of this calculus.
Finally, we study behaviour of Connes' calculus for the multiplication of spectral triples. This problem was investigated earlier by Kastler-Testard but their work appears inconclusive. Hence we reinvestigate this problem and propose a category theoretic conclusion. We cast Connes' definition in a slightly more general algebraic setting and prove that the collection of algebraic spectral triples form a category Spec. It turns out that Spec is a monoidal category and the Connes' calculus is a covariant functor from Spec to DGA, the category of differential graded algebras over a field k. Then we consider a suitable subcategory Spec_{sub} of Spec and prove that restricted to this subcategory Spec_{sub} Connes' calculus is a monoidal functor. To show that this restriction does not lead to triviality of the Connes' calculus we compute it for two cases, namely for a canonical spectral triple associated with compact smooth manifolds and for the noncommutative torus.

Publications

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3. Accepted: Equivalence of Two Approaches to Yang-Mills on Non-commutative Torus, with Partha Sarathi Chakraborty, to appear in Journal of Noncommutative Geometry, arXiv:1304.7616 [math.OA].
4. Submitted: Multiplicativity of Connes' Calculus, with Partha Sarathi Chakraborty, arXiv:1402.5735 [math.QA]

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Title		An Evaluation of Neutronic Safety Characteristics of Prospective Fast Reactor Metal Fuels

Abstract

Due to the increasing demand for electricity in India, fast breeder reactors to be set up beyond 2020 would be based on metal fuels as they have shorter doubling time. Fast reactor cores are not always in a most reactive state and there is always a concern with metal fuel regarding the potential of positive temperature reactivity feedback in accident scenarios. The major temperature reactivity feedbacks are associated with changes in temperature of the fuel (Doppler), structural material (Core radial expansion) and coolant (coolant expansion and voiding). In metal fuel reactors with U-Pu type, one of the major safety concerns is regarding the reduced Doppler feedback and increased sodium void coefficient. It is always preferable to have a large negative Doppler reactivity effect and a negative or near zero sodium void reactivity. The present work tries to identify a fuel type with superior safety characteristics without much penalty on breeding ratio. Transport calculations are carried out taking the exact geometry of the core and using recent nuclear data. It has emerged from this study that the combinations of Th-U fuel type, breeding is not optimal and is not possible for medium sized reactors. Comparative assessment of different candidate fuels is made by considering the actual geometry of the core and arrived at fuel compositions which have superior safety characteristics. ULOFA study of Th-Pu fuel is done for the first time. It emerges from these studies, Th-Pu metal shows the best safety characteristics. The thesis also presents results regarding criticality safety of metal fuels. Estimations on safety limits of fissile mass handling are made for demonstration metal fuel fabrication facility. This study eliminates the possibility of inadvertent criticality in the plant thus ensuring public safety

Publications

Journal:

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2. D. V. Subramanian, A. Haridas, Neethu Hanna Stephen, V. Sathiyamoorthy, C. P.Reddy, R. S. Keshavamurthy (2012), Localization of failed fuel in FBTR, Proc. 19th N SRP conference, Mamalapuram.

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Abstract

In this thesis we have worked on two different directions. In one of them we have explored aspects of joint measurability through an Arthur-Kelly like model for qubits. In the second we have investigated the interrelation between quantum correlation and channels through two different problems.

Firstly,we have considered joint measurement of two and three unsharp qubit observables through an Arthur-Kelly type joint measurement model for qubits. We have investigated the effect of initial state of the detectors on the unsharpness of the measurement as well as the post-measurement state of the system. Particular emphasis has been given on a physical understanding of the POVM to PVM transition in the model and entanglement between system and detectors.Two approaches for characterizing the unsharpness of the measurement and the resulting measurement uncertainty relations have been considered.The corresponding measures of unsharpness have been connected for the case where both the measurements are equally unsharp. The connection between the POVM elements and symmetries of the underlying Hamiltonian of the measurement interaction has been made explicit and used to perform joint measurement in arbitrary directions. Finally in the case of three observables we have derived a necessary condition for the approximate joint measurement and used it show the relative freedom available when the observables are non-orthogonal

In the second part we have investigated qubit channels through their property of 'non-locality breaking', defined in a natural way but within the purview of CHSH nonlocality. This also provides a different perspective on the relationship between entanglement and nonlocality through the dual picture of quantum channels instead of through states. For a channel to be entanglement breaking it is sufficient to 'break' the entanglement of maximally entangled states. We have provided examples to show that for CHSH nonlocality breaking such a property does not hold in general, though for certain channels and for a restricted class of states for all channels this holds.We have also considered channels whose output remains local under SLOCC and called them 'strongly non-locality breaking'. We have provide a closed form necessary-sufficient condition for any two-qubit state to show hidden CHSH nonlocality. Using this we have characterized all strongly non-locality breaking qubit channels. It turns out that unital qubit channels breaking nonlocality of maximally entangled states are strongly non-locality breaking while extremal qubit channels cannot be so unless they are entanglement breaking

Maximally entangled states-a resource for quantum information processing-can only be shared through noiseless quantum channels, whereas in practice channels are noisy. Thus in this thesis we have asked : Given a noisy quantum channel, what is the maximum attainable purity (measured by singlet fraction) of shared entanglement for single channel use and local trace preserving operations? We have found an exact formula of the maximum singlet fraction attainable for a qubit channel and given an explicit protocol to achieve the optimal value. The protocol distinguishes between unital and nonunital channels and requires no local post-processing. In particular, the optimal singlet fraction is achieved by transmitting part of an appropriate pure entangled state, which is maximally entangled if and only if the channel is unital. A linear function of the optimal singlet fraction has also been shown to be an upper bound on the distillable entanglement of the mixed state dual to the channel

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Title		Ultrafast Excited State Dynamics of Intramolecular Charge Transfer Molecules in Solution

Abstract

In this thesis, an effort has been made to understand structure-dynamics relation in photoinduced electronic excited states of various model molecular systems having intramolecular charge transfer character upon photoexcitation. Femtosecond resolved pump probe experiments were performed to measure the excited state dynamics of the chemical systems in real time. The main emphasis has been elucidation of intramolecular charge transfer and proton transfer reactions and associated large amplitude structural relaxation dynamics to discern the role of electronic and geometric factors responsible for the dynamical evolution of the excited electronic states. Effects of solvent polarity, proticity and viscosity have been extensively studied to understand the role of intermolecular interactions and solvent friction in excited state deactivation process. In inorganic systems, intersystem crossing is known to be a general phenomenon which occurs in ultrafast timescale. The rate of ISC and subsequent charge transfer dynamics in inorganic chromophore in triplet manifolds plays crucial role in many applications such as solar energy harvesting. As these processes occur in ultrafast timescale, femtosecond time resolved transient absorption and fluorescence spectroscopy are proved to be efficient techniques to disentangle the complex relaxation dynamics of several competing pathways. The observations made from femtosecond studies on different intramolecular charge transfer molecules have been summarized and the dynamics in photoinduced excited state relaxation have been correlated to electronic and geometric factors. Quantum chemical calculations in excited state employing time dependent density functional theory (TDDFT) were used to substantiate the experimental observations.

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Title		The effect of geometric frustration on some correlarted electron systems

Abstract

The notion of geometric frustration emerged originally in the context of Ising spins with antiferromagnetic nearest neighbour interaction on a triangular lattice. The classic solution by Wannier clarified how long range order is suppressed by frustration in this case. One can generalise the situation to frustrated structures in higher dimensions, e.g, the pyrochlore or the face centered cubic (FCC) lattices, where neighbouring spins live on a tetrahedral motif. Such models, and their classical and quantum Heisenberg versions, have been intensely studied. Correlation physics, on the other hand, grew out of the continuing study of many body systems over the last several decades, with a fresh impetus given by the discovery of high T_c superconductivity in the doped Mott insulator $La_{2-x}Sr_xCuO_4$. This thrust the Mott transition and the doped Mott insulator centerstage. It quickly became apparent that a large family of oxides, including the magnetoresistivemanganites, the high thermopowercobaltates, etc, owed their exotic properties to electron correlation. The development of powerful tools like dynamical mean field theory (DMFT) and its combination with ab initio methods has clarified many aspects of correlation physics over the last two decades.

Correlated systems involve metals systems with itinerant electrons, while traditional frustrated systems are insulating magnets with localised electrons. There are broadly two situations where they intersect:

1. One may have a 'two species' system, of electrons and local moments, where the local moments live on a frustrated structure and are Kondo (or Hund's) coupled to itinerant electrons.
2. We could have a Mott insulator in a frustrated structure and the consider its metallisation, due to decreasing interaction.

The first situation arises in Kondo lattice like, or 'double exchange', models, while the second is described by the Hubbard model. In both cases the ideal frustrated situation arises in the absence of itinerant electrons. The interest is in clarifying how the presence of electrons in the Kondo lattice, or the approach to the insulator-metal transition in Mott-Hubbard systems modifies the physics. The 'two species' description is appropriate for the pyrochlores (iridates, etc) and double perovskites, while the Hubbard model is relevant for materials like the cluster compound $GaTa_4Se_8$ and A_3C_{60}.

The thesis addresses the interplay of correlation effects and geometric frustration in three cases: (i) the metallic double perovskites, (ii) the triangular lattice Hubbard model for the κ-BEDT organics, and (iii) the Mott transition in the face centered cubic (FCC) lattice. Below is the summary of the work presented in the thesis -

Double perovskitesMangetism in double perovskites is driven by electron itinerancy, which can lead to antiferromagnetism. However, in three dimensions the FCC magnetic lattice prohibits Neel order and replaces it with spirals or the flux phase. These have low T_c.
Mott physics We solve the Mott problem through a static auxiliary field approximation implimentedvia Monte Carlo. We (i) uncover non-trivial magnetic correlations on the anisotropic triangular lattice, (ii) study the Mott transition, (iii) highlight the pseudogap DOS and non-drude optical response, and (iv) demonstrate the emergence of the 'hot' and 'cold' spots on the Fermi surface. On the FCC lattice, we (i) observe a spin-glass window near the Mott transition, (ii) the pseudogap persists to zero temperature, (iii) the spinglass window corresponds to very large, finite residual resistivity. This seems to have parallels in the frustrated Mott materials.

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5. Mott transition and glassiness in the face centered cubic lattice.RajarshiTiwari and PinakiMajumdar arXiv:1302.2922

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Title		Cyclic Tearing Investigations on Carbon Steel and Stainless Steel Nuclear Piping Components

Abstract

Currently Leak-Before-Break (LBB) based design and fracture stability assessment considers the earthquake as once applied non-cyclic load, which monotonically increases up to its maximum magnitude. The cyclic character of earthquake load and associated cyclic tearing failure mode (tearing-fatigue regime) are not explicitly considered while demonstrating stability of a through wall cracked pipe. In past, huge efforts and investigation were made to understand, quantify and develop procedure to account for the load history effect, reversible cyclic loading into the fracture stability assessment while demonstrating the leak before break behaviour of a cracked pipe. These investigations have shown the deleterious cyclic tearing damage under a cyclic loading event. Despite the efforts, the cyclic tearing failure mode is not explicitly accounted for in present guides/practices of stability demonstration of a cracked pipe for LBB analyses. This may be due to un-availability of simple, reliable and easily implementable procedure to demonstrate the fracture stability of cracked pipes for specified number of cycles as required in level-3 of LBB analysis.

A systematic focused experimental study has been carried out to single out and quantify the deleterious effect of the cyclic character of applied load on stability assessment of a circumferential through wall cracked pipe. The test program involved extensive number of cyclic tearing and corresponding monotonic fracture tests on large sized pipe components. Tests have been conducted on seamless pipes made from carbon steel (CS of SA-333 Gr.6) and austenitic stainless steel (SS of SA-312 Type 304LN) material. The CS is the material of the Primary Heat Transport (PHT) system piping of Indian Pressurized Heavy Water Reactors (IPHWRs) while the SS is the proposed material for the Main Heat Transport Piping (MHT) system of Indian Advanced Heavy Water Reactor (AHWR). The tests have been carried out on pipes of two different base material (SSB and CSB) and three different girth weld configurations/combinations. The circumferential through wall notch was machined at weld centre line of the girth welded pipe and in base metal at centre of actual pipe. The girth welded pipe specimens were prepared by joining two seamless pipe pieces using two different welding techniques namely Shielded Metal Arc Welding (SMAW) with conventional groove (CSW and SSW) and Gas Tungsten Arc Welding (GTAW) with narrow Groove (NGW). The NGW procedure is the proposed welding technique for stainless steel piping of AHWR. The pipes specimens named as CSB, CSW, SSB, SSW and NGW, are regarded as five material categories and covered reasonable variation in fracture toughness. A

series of monotonic fracture tests have also been conducted to obtain the base line data under monotonically increasing load conditions corresponding to each cyclic tearing test. The pipe size, material, crack size and crack location used are identical in cyclic and monotonic fracture tests. These tests covered reasonable variation in pipe size, crack size, crack location, load history, loading control type, weld techniques and nuclear piping material etc. The piping system is subjected to mixture of load controlled and displacement controlled conditions. Therefore, the cyclic fracture tests were done under both the pure load controlled as well as pure displacement controlled loading conditions. In addition to these, limited data on similar tests on STS410 Japanese carbon steel has also been included in current investigation.

The displacement controlled cyclic tearing tests of all five material categories along with corresponding monotonic fracture tests on identical pipes, have been analysed. The displacement Ph.D. Thesis entitled “Cyclic Tearing Investigations on Carbon Steel and Stainless Steel Nuclear Piping Components” by Suneel Kumar Gupta controlled cyclic loading tests shown very high tearing crack growth leading to DEGB under step wise build-up of cyclic displacement loading. The relative comparisons of the pipe fracture behaviour obtained from cyclic displacement and corresponding monotonic fracture tests. A small decrease in the maximum moment but large decrease in corresponding displacement value is observed when compared to those obtained in monotonic fracture test on identical pipe. The cyclic J-R curves of all five material categories have shown significant decrease in fracture resistance under cyclic loading conditions. Smaller the cyclic displacement increment step resulted in larger drop in cyclic J-R curve. The load controlled cyclic tearing tests have been conducted to assess the pipe crack growth and fracture stability behaviour during an earthquake event and they in general are treated as load controlled and of fully reversing cyclic in nature. They revealed that the pipe may fail by unstable tearing in very few cycles under fully reversible load with a magnitude much below the monotonic capacity of pipe. The unstable failure of pipe us preceded by large crack growth. The crack growth and number of cycles before unstable failure are found correlated with applied loading. Larger compressive load in reverse direction (that is when larger negative load ratio) caused cyclic damage and resulted in accelerated crack growth.

Each of the load controlled cyclic tearing test results have been assessed in relation to corresponding monotonic fracture test conducted on identical pipe. The effect of number of load cycles and cyclic tearing damage on stability of a pipe is quantified in term of a load reduction factor (□). The □ factor is defined as ratio of magnitude of cyclically applied load to the load capacity of the identical pipe under monotonically increasing load. A Cyclic Tearing Failure Assessment Diagram (CTFAD) is developed from □ factors. A lower bound CTFAD curve equation (□L) is proposed for fracture stability assessment under cyclic loading. The □L factor usage enables the existing procedures of stability assessment to demonstrate the integrity for specified number of load cycles. Based on CTFAD and proposed equation, load reduction factors are proposed to rule out the unstable failure of a cracked pipe for different number of load cycles associated with different levels of earthquakes.

The thesis has been structured into seven chapters. The scope and significance of the research and the motivation behind the present investigation are briefed in Chapter-1. The salient literature background related to the current investigation has been presented in Chapter-2. The Chapter-3 presents details of the experimental program, methodology, and salient results. Chapter-4 presented the investigation on the cyclic / monotonic J-R curves and the pipe fracture behaviour under displacement controlled cyclic loading. The pipe fracture stability and crack growth behaviour under load controlled conditions are discussed in Chapter-5. The Chapter-6 presented how the cyclic tearing damage is quantified and singled out from other aspects which affect the fracture stability behaviour of pipe. A cyclic fracture stability assessment method is proposed here. An overview of the conclusions derived from this work has been summarized briefly in Chapter-7 together with some proposed future work related to this area. All references quoted throughout the dissertation have been given after Chapter-7. Ph.D. Thesis entitled “Cyclic Tearing Investigations on Carbon Steel and Stainless Steel Nuclear Piping Components” by Suneel Kumar Gupta

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Title		Rotation Curve of the Milky Way and the Phase-Space Structure of its Dark Matter Halo: Implications for Direct Detection of Weakly Interacting Massive Particle Candidates of Dark Matter

Abstract

Detetion of dark matter (DM), whih onstitutes ∼ 26% of the present energy density in our Universe, has been one of the toughest hallenges in astropartile physis for severaldeades. In order to analyze and interpret the results from DMdiret detetion (DD)searh experiments, one needs tworuial astrophysial inputs, namely, the loal (i.e.,theSolar neighborhood) density of DM (_DM,⊙) and the loal veloity distribution funtion(VDF) of theDM partilesonstituting the Galatihalo, whih areurrently not knownwithertainty. Towards this end, in this thesis, we attempted to derive these quantitiesfrom RC data, pertaining to the MilkyWay. First, we have studied the `isothermal sphere'(IS) modelustomarily used in the soalled `standard halo' model (SHM) desription ofthe phase spae distribution funtion (PSDF) of the DM partiles (assumed to be`WeaklyInterating Massive Partiles' or WIMPs throughout this thesis). We have found

that,byonsidering the e_et of the gravitational in_uene of the visible matter (VM), theIS halo requires values of DM veloity dispersion, hv2i1/2,onsiderably higher than 270kms−1, a valueustomarily adopted in the `isolated' SHM model along with _DM,⊙ ≃ 0.3GeVcm−3, to _t the RC data. The DDompatibility region in the WIMP mass versusross-setion parameter spae signi_anthanges with inreasing values of hv2i1/2 andwith WIMP-nuleus sattering inelastiity parameter. However, the IS su_ers from someserious limitations in providing a realistidesription of Galatihalo. We have, therefore,onsidered the `King' model, another solution ofollisionless Boltzmann equation like theIS model, desribing a spherially symmetriored_nite size PSDF of the Galatihalo.The parameters of the models have been determined by_tting the observed RC data of ourGalaxy by inluding the e_et of gravitational in_uene of the observed VM on the PSDFdesribing the DM halo in a selfonsistent manner. The gravitational in_uene of VMhas a signi_ant e_et in _pulling in_ more DM towards theenter of the Galaxy leadingto a shrinking of theore radius by enhaning theentral DM density and introduing a_attening of DM density on the disk by 30-40%. The VDF is non-Maxwellian in naturewith a sharput o_ at a _nite maximum speed and has signi_ant e_et on the best _tDAMAompatible regions lying in 2-16 GeV rangeompared to results in theontext ofSHM, whih has a a typial Maxwellian VDF. We have presented aomprehensive studyof the derivation of the _DM,⊙, using RC data of our Galaxy extending up to ∼ 200 kpc forvarious GalatiConstants (GCs) sets, by adopting four di_erent pro_les for the GalatiDM halo model. We have found that the best _t _DM,⊙ is fairly independent of the DMhalo density pro_le (be itored oruspy) and it varies from ∼ 0.2 to ∼ 0.6 GeVcm−3(by a fator of ∼ 3) for theirular veloity of the loal standard of rest frame aroundthe Galatienter (V0)hanging from 200 to 244 km/se. We have next derived thePSDF of the WIMPs by _inverting_ the best _t Einasto density pro_le using Osipkov-Merritt formalism inluding the e_et of the gravitational in_uene of VM on DM in aselfonsistent manner. The PSDF so obtained isharaterized by an anisotropiveloityspae with a lower bound on anisotropy radius as 4 kpc (with loal anisotropy parameter≤ 0.81). The e_et of gravitational in_uene of VM is signi_ant up to ∼ Solar radius andfound to support higher radial and tangential values and introdue an additional broadpeak in the inner Solarirle region for the veloity dispersions. However, the VM e_etdereases with higher radii, as expeted. We have also attempted theonstrution of theRC data of our Galaxy without referring toanyspei model of the VM or DM haloof the Galaxy byonsidering kinematial data on a variety of disk traer objets. Wehave investigated the sensitivity of the disk RC data with the assumed set of GCs and found that, at any given position, theirular veloity is higher for higher value of V0.Our _ndings, presented in this thesis, have signi_ant impliations for the analysis andinterpretation of the results of DD experiments, whih we propose to study in more detailin future.

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Title		Simullation of In-Vivo Monitors and Voxel Phantoms for Establishing Calibration Factors

Abstract

Physical phantoms representing typical Indian is an essential requisite for any in vivo monitoring program in India which presently depends on phantoms representing western men. This is because the differences in the anatomical and physiological characteristics between the various populations can result in large uncertainties in the calibration factors leading to erroneous quantitative assessment of the internal contamination and the consequent dose estimation especially for low energy photon (LEP) measurements. For High Energy Photons (HEP) measurements a few Indian reference phantoms have been developed. These physical phantoms still represent the standard reference man and have large limitations in terms of its use in experiments to study the influence of human morphology, variation in source distribution etc. Moreover, there is no realistic physical phantom for both male and female for the calibration of monitors used for actinides measurements. Developing numerical simulation techniques specific to each laboratory can solve the above mentioned problems.

This dissertation focuses on the modelling and simulation of in vivo monitors and voxel phantoms for establishing calibration factors. To accomplish the desired task, all the in vivo monitors at IGCAR have been theoretically simulated with the virtual models of the physical phantoms available and validated against experimental results. The validated models were applied to estimate the calibration factors for new geometry, various sizes, specific organ of radionuclide deposition for which the physical phantoms are not available, etc. The influence of variation in source distribution, body physique and detector placement etc., on the calibration factors have also been studied. Significant findings of this dissertation include; (i) indigenously developed cost effective Masonite cut sheet phantom is a good substitute for Indian BOMAB phantom in the high energy regions (>200 keV), (ii) distribution of six numbers of Natural Uranium source plugs in the center of each lung of LLNL phantom is equivalent to the uniform distribution for single Phoswich based lung measurement, (iii) calibration factors are estimated for Phoswich detector for ^{239}Pu present in the lungs, for female subjects and calibration factor of thin NaI(Tl) detector for bone seeking radionuclides deposited in the knee. Lung measurement using single Phoswich detector and knee measurement using 5cm diameter NaI detector are unique to IGCAR, WBCF. To estimate the calibration factors for ^{241}Am deposited in the skull, physical phantom is not available at IGCAR. Skull voxel phantoms have been developed from the CT images to estimate the same. The focused studies have clearly validated procedures, techniques, provided calibration factors and greater insights. But there is still some scope which includes quantification of the interference from the ribs on the lung measurement and estimating the calibration factors for non- standard counting geometries using the developed counting systems numerical model.

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Publication not related to this thesis work

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2. Manohari M., Mathiyarasu R., Rajagopal V. and Meenakshisundaram V. Testing of in situ emergency monitoring field instruments with a subject undergone medical diagnostic testing. Proceedings of International Symposium on Accelerator and Radiation Physics (ISARP-2011), February 16-18, 2011, Saha Institute of Nuclear Physics, pp.268-271.
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Abstract

During my doctorate work, I have studied various aspects of neutrinos at extremely high energies (10 TeV and higher), specifically with a view to unravelling possible hints of nonstandard physics that might be embedded in such events. Neutrinos at energies greater than 10 TeV are produced in the extremely energetic cores and jets of astrophysical sources located either within our galaxy (e.g. pulsars, supemovae, etc.) or outside our galaxy (e.g. active galactic nuclei (AGN), gamma ray bursts (GRB), etc.). Thereafter, being extremely inert, they stream to the earth almost unperturbed, with only oscillation among the three flavours modifying their fluxes. Because the fluxes of the neutrinos produced at these energies are extremely low, detecting them at the earth requires detectors with very large volumes (1 km^3). The IceCube (IC), built at the South Pole into the Antarctic ice bed, is a 1 km^3 detector designed to detect and study such high energy neutrinos. My work has involved analysing the neutrino events that might be seen at IC, in the future, to understand:

- The nature of the source producing these neutrinos,
- The nature of mixing among the three flavours as the neutrinos oscillate while propagating from the source to the earth, specifically looking at whether it is in keeping with standard physics or affected by small non-standard physical effects such as neutrino decay, violation of Lorentz invariance, etc., and
- Novel signatures of the highest energy standard model process hitherto unseen, viz. the Glashow Resonance (GR), occurring when an electron-antineutrino with energy of 6.3 PeV (in the lab frame) interacts with an electron within the IceCube resulting in the production of W~ at resonance, which then decays promptly into hadrons and, to about one-sixth of the time, into leptons.
-

IceCube is capable of distinguishing between the three flavours of neutrinos, as they interact with the nuclei within the detector, by means of their event topologies:

- Showers due to charged current interactions of the electron-neutrino and, for incident energies less than a PeV, tau-neutrino, and, neutral current interactions of all the three flavours,
- Muon-track events due to the charged current interactions of muon-neutrinos, and finally
- Signature topologies of the tau-neutrino at energies above a PeV, such as the double bang, lollipop, etc.

In my work with my supervisor and other collaborators, we have shown that, as IceCube collects a significant number of events over the next five years, it will be possible, by comparing the fluxes of three flavours, to detect signatures of non-standard physics, if any, on the neutrino oscillation probabilities at these energies. By considering each of neutrino decay, Lorentz violation, existence of additional pseudo-Dirac neutrinos and quantum decoherence in turn, we have predicted the expected parameter space in each case that such high energy events will be sensitive to, and should therefore be able to rule out if the events are consistent with expectation from standard physics.
Finally, we have also discussed the possibility of seeing the GR in the IceCube. Specifically we have calculated the expected number of shower events around the GR energies, at 6.3 PeV as a function of the source spectrum and discuss the rare but tell-tale and completely background-free events seen when the resonantly produced W decays to leptons, rather than to hadrons. We have also shown how non-standard physical effects might modify the number of events otherwise expected around the GR energies.

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Journal

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Title		Study of Transformation Characteristics and Micro-Structural Evolution in 9Cr Reduced Activation Ferritic/ Martensitic Steel Using Electron Microscopy, Calorimetry And Computational Methods

Abstract

Reduced activation ferritic / martensitic steels with W and Ta substitution in modified 9Cr steels are considered for the structural materials for Test Blanket Module of future fusion reactors. My thesis work involves the study of effect of W and Ta on Phase Transformation characteristics and microstructural changes under thermal aging and creep deformation. Various microstructural parameters of these steels Prior Austenite Grain Size, martensite lath width and fine second phase carbide precipitation w.r.t their microchemistry and distribution in the matrix have been characterized extensively with different microscopy techniques especially Scanning and Analytical Transmission Electron Microscopy. The observed microstructural changes were correlated to the hardness measurements to understand the effect of alloying elements on strength of the steels. The transformation sequence in the steel was established using differential scanning calorimetry technique. The observed transformation sequence was supported by JmatPro simulations.

Orientation imaging of normalised 1.4W steel was performed to study the martensite characteristics. A low amount of retained austenite (~2%) was detected by the phase map and the Mossbauer Spectroscopy.Detailed investigation of the microstructure performed in Phlips CM-200 ATEM fitted with X-max SDD detector showed the presence of fine acicular carbides of the size 5 to 10 nm in steels containing higher amount of W. A systematic study of microstructure microchemistry and selected area diffraction patterns were used to identify and quantify the observed precipitates. As power plant steel enters in to service at high temperature, it is adequate to have a stable microstructure rather than a martensitic microstructure. It is highly recommended to temper the steel before using in actual service mode. In this respect, the study of tempering kinetics was essential. In present study, the activation energy for the tempering of martensite was estimated using hardness measurement and XRD analysis. TEM investigations of the samples after tempering showed the presence of $M_{23}C_6$ and MX precipitates with the systematic variation of size and number density with W and Ta content of the steel.

Studies on long term thermal stability was also performed to understand the effect of thermal and stress exposure. Microstructural results from TEM were used to identify and quantify the phases evolved in the steel during thermal exposure. Proofs and evidences from chemical mapping were compared with the composition simulated by JmatPro.

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2. Influence of W and Ta content on microstructural characteristics in heat treated 9Cr-Reduced Activation Ferritic / Martensitic steels, Ravikirana, R. Mythili, S. Raju, S. Saroja, T. Jayakumar, E. Rajendrakumar, Mater. Charact., 84 (2013) 196 – 204.
3. Effect of alloy content on microstructure and microchemistry of phases during short term thermal exposure of 9Cr-W-Ta-0.1C Reduced Activation Ferritic/Martensitic (RAFM) steels, Ravikirana, R. Mythili, S. Raju, S. Saroja, G. Paneerselvam, T. Jayakumar, E. Rajendra Kumar, Bulletin Mater. Sci., 37 (6) (2014) 1453–1460.

4. Decomposition Modes of Austenite in 9Cr-W-V-Ta Reduced Activation Ferritic Martensitic Steels, Ravikirana, R. Mythili, S. Raju, S. Saroja, T. Jayakumar and E. Rajendra Kumar, Mater. Sci. Tech., 31 (4) (2014) 448-459
5. High Temperature Phase Stability of 9Cr-W-Ta-V-C Based Reduced Activation Ferritic-Martensitic (RAFM) steels: Effect of W and Ta additions, Ravikirana, S. Raju, R. Mythili, S. Saroja, T. Jayakumar and E. Rajendra Kumar, Steel Res. Int.,(2014) doi:10.1002/srin.201400183.

II. Manuscript under preparation

1. Evolution of secondary phases in 9Cr RAFM steels with varying W, Ta content - Experimental and computational studies
2. Identification of retained austenite in normalised 9Cr RAFM steels

III. Conference Proceedings

1. Effect of heating rate on transformation temperature of 9Cr-W TaV RAFM steels, Ravikirana, S. Raju, R. Mythili, S. Saroja, T. Jayakumar and E. Rajendra Kumar, Proc. 19th Symp. on thermal analysis (Thermans -2013), Mumbai, India, 2013, pp.414 – 419.
2. Effect of alloy content on microstructure and microchemistry of phases during short term thermal exposure in 9Cr-W-Ta-C RAFM Steels, Ravikirana, R. Mythili, S. Saroja, T. Jayakumar, E. Rajendrakumar, Proc. ISRS-2012, Chennai, December 13-15, 2012, 1.
3. Microstructural modifications due to W and Ta in 9Cr Reduced Activation Ferritic / Martensitic steels on creep exposure, R. Mythili, Ravikirana, J. Vanaja, K. Laha, S. Saroja, T. Jayakumar, M.D. Mathew, E. Rajendrakumar, Proc. 6th Int. Conf. on Creep, Fatigue and Creep-Fatigue Interaction (CF-6), Mamallapuram, India, January 22-25, 2012, pp.685-689.

IV. Conferences

1. Study of precipitation kinetics in W added 9Cr- RAFM steel, R. Mythili, Ravikirana, S. Saroja, 48th NMD-64th ATM, Nov.14-17, 2010, Bengaluru.
2. Study of microstructural evolution in 9Cr Reduced Activation Ferritic / Martensitic steels under the influence of temperature and stress, Ravikirana, R. Mythili, J. Vanaja, K. Laha, S. Saroja, 49th NMD- 65th ATM, Nov. 13-16, 2011, Hyderabad.
3. Role of W and Ta on transformation characteristics and microstructure development in 9Cr-W-Ta-C RAFM Steels, R. Mythili, Ravikirana, S. Raju, S. Saroja, T. Jayakumar, M.D. Mathew, E. Rajendrakumar, IAEA Topical Meeting, December 11-13, 2012, Gandhinagar.
4. Study of $\gamma \rightarrow \alpha'$ transformation in 9Cr-ferritic martensitic steel by Automated Crystal Orientation Imaging Microscopy, R. Mythili, Ravikirana, L. Herojit Singh, R. Govindaraj, S. Saroja and M. Vijayalakshmi, 52nd NMD- 68th ATM, Nov. 12-15, 2014, Pune, India.

Annex 5
Titles of M.Tech., M.Sc. (Engg.) & M.Phil. Theses for which results were notified during April 1, 2014 to March 31, 2015

Titles of M.Tech. Theses for which results were notified during April 1, 2014 to March 31, 2015

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
1	Nitesh Goswami	15.04.14	Evaluation of Membrane Reactor for III Decomposition Studies
2	Moushumi Datta Chaudhury	21.04.14	Uncertainty Analysis of Transport Model of Tritium in Atmosphere-Soil-Plant System and Formation of Organically Bound Tritium
3	Vijay Kumar Sohani	21.04.14	Nonlinear Schrodinger Equation and the Twisted Laplacian
4	Satyabrata Mishra	21.04.14	Studies on Development of Process Related Issues in Aqueous Reprocessing of Fast Reactor Spent Fuels
5	Rabindra Nath Juine	23.04.14	Silver Doped ZnS Nanomaterial and its Various Applications as Detector Material
6	Saurabh	29.04.14	Modelling of Spray Drying Process for Zero Liquid Discharge (ZLD) Desalination System
7	Sudipan De	12.05.14	Photon Production and Forward-Backward Multiplicity Correlation in Alice at the LHC
8	Tanumoy Mandal	12.05.14	Phenomenology and LHC Signatures of Exotic Fermions
9	Vandan Nagar	12.05.14	Molecular and Biochemical Studies of *Aeromonas SPP*
10	S. Sukumar	12.05.14	Synthesis and Characterization of Substituted Hydroxamic Acid and its Performance in the Separation and Purification of Pu and U
11	Satya Rajesh Medidi	12.05.14	Design of Fine Impulse Test System for SCRAM Logic System
12	Sagar Chandra	26.05.2014	Understanding the Macroscopic Shape Change through Multiscale Modeling of Deformed Copper Single Crystals
13	Naisheel Verdhan	26.05.2014	Interaction of Dislocations with Boundaries using Discrete Dislocation Dynamics
14	Lijukrishnan P.	28.05.14	Development and Optimizatio;n of Gas Entrainment Mitigation Devices for Surge Tank of Future FBR
15	Pidapa Raghava Reddy	02.06.14	Modeling, Simulation and Integrated Testing of Turbo Generator Auxilliary System of PFBR
16	Jitendra Singh	02.06.14	Characterization of Various Transit Compositions for Development of Transitions Joint Between Titanium and Type 304L Stainless Steel with Ni Interlayers
17	Alok Prakash	11.06.14	Development of Phased Array Ultrasonic Technology for NDE of Weld Joints in Shell and Hydro-Chamber Assembly of Compact Steam Generators
18	Amitanshu Mishra	02.07.14	Simulation of Multiple Loop Channel Type Natural Circulation BWR for Cold Start-up

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
19	Ashutosh Shivhare	16.07.14	Development of Manufacturing Method and Numerical Simulation of Deformation of Dumb-Bell Shaped Tube
20	Muneer M.P.	23.07.14	Nuclear Power Plant Emergency Power Supply System Diesel Generator Reliability Modeling and Analysis
21	Kamath Sachin Vasant	24.07.14	Modeling & Simulation of Alkaline Water Electrolyzer with Porous Electrodes
22	Anand Mitra	24.07.14	Tomographic Image Reconstruction using Graphical Processing Unit (GPU) for Industrial Non-Destructive Examination (NDE)
23	Chandra Prakash Kewat	30.07.14	Study of Stratification and Conjugate Heat Transfer Behaviour for Low Reynolds Number in Tubular Geometry
24	Arvind Singh Padiyar	04.08.14	Development of Transition Joint Between Titanium and AISI Type 304L Stainless Steel
25	Tushar Sharma	07.08.14	Determination of Axial Thrust on the Impeller of a Vertically Mounted Centrifugal Pump using CFD Analysis
26	Vikas Jain	13.08.14	Design and Development of a Low Voltage Distribution System for High Energy Physics Detectors
27	Suvadip Roy	16.08.14	Feeder Pipeline Wall Thickness Measurement Using Pulsed Eddy Current Technique
28	Garima Pandey	16.04.14	Mass Transfer Studies on Recovery of Zirconium and Hafnium from Zirconium Oxide Plant Raffinate Using Solvent Extraction
29	Ananya Monanty	16.08.14	Study of Buoyant Hydrogen Jet in Stratified Atmosphere in a Multi-Compartment Enclosure of Containment Study Facility
30	Baribaddala Ravi	16.08.14	Design and Development of Automatic Exposure Control Monitoring System for Digital Medical Imaging System
31	Ankita Agarawal	16.08.14	Development of Thermal-Hydraulic Model for Analysis of Passive Autocatalytic Recombiner
32	Rohit Sinha	22.08.14	Effects of High Viscous Dampers on the Dynamic Response of Underground Hardened Structure Subject to Surface Blast
33	Md Tipu Sultan	25.08.14	Theoretical and Experimental Investigation of Thermal Valves for Core Catcher System (CCS) of AHWR
34	Kumar Rahul	25.08.14	Interaction of Rotating Machinery with Structures and Equipment under Seismic Loading
35	Nishant Mishra	28.08.14	Motor Current Signature Analysis for Fault Detection in Three Phase Squirrel Cage Induction Motor using Wavelets

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
36	Ramandeep Singh Sawhney	02.09.14	Strain Development at Weld Fusion Zone and Base material Interface: Narrow Gap Vs Manual GTAW Type of Welds
37	Mukade Suraj Kalyanrao	02.09.14	Fault Tolerant Network Management System
38	Vinayak Sharma	02.09.14	Safety Analysis Under Accident Condition of Lead Shielded Transfer Cask
39	Romali Biswal	02.09.14	Development of Pressurized Capsules with Attachment of Central Thermocouple for Detection of Creep Rupture in Fast Reactor Clad Tubes
40	Santosh Kumar Tiwari	19.09.14	Effect of Hydrogen Content and Hydrides on the Oxidation Behaviour of Zirconium Alloys
41	Harshad Shivaji Tarate	19.09.14	Stress Corrosion Cracking of Stainless Steel Grade 304 L in Chloride Environment - Effect of Oxygen and Potential
42	Prafful Kumar Sinha	19.09.14	Effect of Microstructure on Oxide Formation on Carbon Steel in Hot Conditioning Simulated Conduction
43	Pratanu Chakraborty	19.09.14	Beam Dynamics Study and RF Design Optimization of Superconducting Quarter Wave Resonators from 1 to 2 MeV/u for VECC RIB Facility
44	Ajay Kumar	19.09.14	Vulnerability Assessment of USB-Based Storage Devices in Networked End System
45	Rinson Antony T.M.	19.09.14	Design and Development of Two Axis Control and Drive for PMSM Motor of In-Service Inspection Module for PFBR Steam Generator
46	Hitendra Yadav	25.09.14	Low Power RF Measurements, High Power Conditioning, X-ray Measurements & Commissioning of Two 37.8 MHz Re-Buncher Cavities
47	Pew Basu	25.09.14	Uncertainty Estimation of ^{40}K Content in Dietary Intake Samples Around Kalpakkam
48	Amit Kumar	25.09.14	Design and Simulation of Wall Current Monitor for Accelerator Instrumentation
49	Himanshu Sharma	07.10.14	Theoretical Investigation and CFD Analysis of Centrifugal Liquid-Solid Clarifier
50	Mohammad Soharab	10.10.14	Growth and Investigation of Yb:YVO_4 and Co-Doped Yb:YVO_4
51	Pankaj Kumar	10.10.14	Quench Analysis for 9T Superconducting Solenoid Magnet
52	Jyoti Sharma	13.10.114	Studies on Nd: Glass Based Laser Amplifiers for High Power Laser System
53	Baidurjya Nath	22.10.14	Characterization & Treatment Study of Thorium Bearing Effluent

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
54	Aniket Chowdhury	22.10.14	Raman Spectroscopic Investigation of Trap Beam Power Dependent Oxy-Deoxygenation of Optically Trapped Red Blood Cells
55	Sandhya Mohanan	22.10.14	Design and Development of Borehole Deviation Measurement System for Uranium Exploration
56	Mani Kumar	22.10.14	Development of Containment Transport Model for Groundwater Using Site Specific Parameters at Challekere
57	Sona Chandran P.	27.10.14	Study of Transport of Low Energy, Space Charge Dominataed Electron Beam in FELs and Design of Magnets for Improved Beam Transport in IRFEL
58	Srijan Kumar	27.10.14	Seismic Response Control of Stiffness Mass Asymmetric Benchmark Structure Using Semi-Active Devices
59	Abhishek Sharma	27.10.14	Studies on Stripping of Uranium in Dispersion Liquid Membrane System in a Hollow Fiber Contractor
60	Vikas Rai	27.10.14	Synchronization of High Pressure Laser Triggered Spark Gaps
61	Manish Pathak	30.10.14	Modeling and Simulation of Inductively Coupled Plasma Generation for RF External Antenna Based H* Ion Source
62	Kriti Pathak	30.10.14	Analysis and Design of a Pulse Power Solid State RF Amplifier
63	Sandeep Kumar	30.10.14	Mathematical Modelling of Ammonia Cracker in Mono-Thermal NH_3-H_2 Exchange Process
64	Nayak Anil Sadananda	30.10.14	Design and Development of Solid State Based High Voltage Pulsed Power Supply with High Repetition Rate
65	Rahul Rana	05.11.14	Design and Analysis of Model Predictive Control (MPC) for Fast Orbit Feedback Control System
66	Meghnath Sen	11.11.14	Design and Development of a Portable Transfer Standard for the Neutron Source Yield Measurement
67	Ambuj Kumar Singh	11.11.14	Vapor Liquid Equilibrium Data Generation of TBP-NDD/NPH at Different Pressure and Correlating Them with Suitable Thermodynamic Model
68	Amrit Pal Singh	11.11.14	Groundwater Migration Studies of Natural Uranium from Solid Waste Disposal Facility at NFC Hyderabad Using Site Specific Parameters
69	Vandana Chaturvedi	11.11.14	Studies on Reaction Sintering of Yttrium Aluminium Garnet (YAG)
70	Jyothi Sharma	11.11.14	Evlaution of LSCM (La-Sr-Cr-Mn oxide as an Interconnect Material for Solid Cell and its Integration with Porous Electrodes
71	Anchal Bakiwala	11.11.14	Studies on Thermal Stratification in Water Pool Using Simplified Mathematical Approach and its Validation with Experimental Data

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
72	N. Sathish	11.11.14	Design and Development of Fire Detection System for Zirconium (Zr) Fire and Zirconium Chloride ($ZrCl_4$) Fumes Using Real Time Video Processing
73	Pravin Prakash Yerunkar	11.11.14	Reliabillity Based Evaluation of Ground Vibration Parameters for Design of Underground Structures Subjected to Blast Loading
74	Brajesh Kumar Jha	11.11.14	Configuration, Analysis and Embedded System Design of Sinusoidal Pulse Width Modulation
75	Ram Prakash	11.11.14	Studies on Modelling of Multipacting in Superconducting Accelerating Cavities
76	Ratnesh Pal	13.11.14	Pulse Height Analyzer (PHA) Implementation on Programmable System on Chip (PSoC)
77	Sadhvi Srinivasan	23.11.14	Experimental Studies on the Reduction of U_3O_8 in an Atmoshere of Ammonia to Produce UO_{2+x} with Higher Density
78	Shibashankar Das	23.11.14	Investigation of Fracture Resistance Behaviour of Nuclear Reactor Fuel-Clad Tubes Using Non-Standard Specimen Tests and Finite Element Analysis
79	Asif Ahmad Bhat	23.11.14	Experimental Simulationj of Mixing of Two Fluids with Large Density Difference
80	Ronie Adhiraaj Ghosh	27.11.14	Development of Laser Based Level Measurement Sensor for Liquid Level Measurement of ADSS Experimental Loop
81	P.M. Dinesh	27.11.14	Strain and Load Controlled Fatigue Behavior of 321 Stainless Steel at 633 K
82	Serai Prashant Prathamesh	28.11.14	Mobile Robot Localization in the Presence of Unexpected Static and Dynamic Objects in the Environment
83	Vivek Singh	03.12.14	Modelling and Performance Analysis of Operation Grade Decay Heat Removal System
84	Deepika Vinod	10.12.14	Design and Development of Solar Powered WSN Sensor and Router Nodes
85	Sandeep Kumar Jaiswal	10.12.14	Study on Recovery of Nitric Acid from Aqueous Acidic Solution in Presence of Nitrate Ions
86	Priyanka Wadhawan	10.12.14	Simulation Modelling for Performance Analysis of PC-AE-1553 Network
87	Arup Singha Roy	17.12.14	Design Optimization of Plastic Scintillator Based Flow-Cell for Tritium Monitoring
88	Anurag Samantara	30.12.14	Investigation of Coupled Natural Convection Loops in Decay Heat Removal Systems of Fast Breeder Reactors
89	Tanumay Bhattacharya	30.12.14	Analytical and Numerical Study of Temperatura Distribution for End Cap Resistance Upset Welding and Experimental Validation

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
90	Vishnu Narayanan K.I.	30.12.14	Study of Hot Radial Forging of Zr2.5%Nb- Simulation and Validation
91	Gunisetty Swathi	30.12.14	Study and Simulation of Electromagnetic Fields Around Power Equipment, in Nuclear Fuel Complex
92	Rahul Arya	30.12.14	Design of Observer Based State Feedback Controller for Advanced Heavy Water Reactor
93	Aswin S. Prabhu	30.12.14	Study, Evaluation and Implementation of Loop Current Step Response Algorithm in a Portable Instrument for the In-situ Calibration of RTDs
94	Vijay Singh Sikarwar	14.01.15	Prediction and Validation of Impurity Precipitation Pattern Over the Wire Mesh of Integrated Cold Trap
95	Sinisetti Venkatanaga Ayyappa	14.01.15	Hydrodynamics and Mass Transfer Studies in a 50mm Centrifugal Extractor
96	Jithu P.G.	18.02.15	Mathematical Modeling and Simulation of Fluorine Production System
97	Gangishetti Saikrishna	24.02.15	Machine Vision Based Dimensions Inspection System for Spacer Pads and Bearing Pads of PHWR Fuel Bundle
98	Rohit Sharma	24.02.15	De-Noising of Low Intensity Fluorescence Signal
99	Pavi Gupta	24.02.15	Prediction of Thermal Hydraulic Behaviour of Lead Bismuth Alloy and Comparison with Sodium
100	Shivangi Agarwal	24.02.15	Experimental Study on Effect of Hydrogen Concentration and Test Temperature on Fracture Toughness of Zr-2.5Nb Pressure Tube Manufactured Employing Double Radial Forging and Single Pass Cold Pilgering
101	Mohit Narang	24.02.15	Study of Ultrasonic Inspection of Improperly Oriented Defects in PHWR Endcap Welds
102	Suheel Shafi	09.03.15	KINETIC STUDIES ON ION EXCHANGE OF FISSION PRODUCTS INTO SYNTHETIC ZEOLITE 4A
103	Ravindra Singh Rawat	09.03.15	Radioactive and Thermal Hydraulic Studies of Heavy Liquid Metal Spallation Target for Accelerator Driven System
104	Atyam Swami Naga Pavan	09.03.15	SOLVENT WASH STUDIES TO REMOVE DEGRADATION PRODUCTS OF TBP
105	Pusapati V.S.N. Prudhvi Raju	09.03.15	Study on the Effect of Free Acidity and Entrained TBP in UNPS on Quality of ADU
106	Rajendra Singh Shekhawat	09.03.15	Studies on the extraction behavior of Gadolinium with Tri-Butyl Phosphate
107	Yatindra Kumar	19.03.15	Creep Crack Growth Characterization of P91 Steel Welds

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
108	Vishnu Mohan T.	19.03.15	Diluted Wash Studies for the Removal of Dissolved TBP in Purex Process
109	N. Anil	19.03.15	Design and Development of Analog Input module for the Airborne Data Acquisition System of Tiome Domain ElectroMagnetic (TDEF) System
110	Darshan N. Pajithaya	19.03.15	Development of a Steady state Code for a Vertical Tube In-pool Condenser
111	Seepika	25.03.15	Methodology for Identification of Static and Dynamic Exposures of TL Personnel Dosimeters for Low Energy Protons
112	Ankit Agarwal	31.03.15	Study on Effect of Strain Path on Properties of Pilgered Tubes

Titles of M.Sc.(Engg.) Theses for which results were notified during April 1, 2014 to March 31, 2015

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
1	K. Mariappan	02.06.14	Estimation of Residual Low Cycle Fatigue Life from Tensile Properties of SS 316L(N) and Modified 9Cr-1Mo Ferritic Martensitic Steel
2	Dandekar Nitin Kamlakar	28.01.15	Experimental Study and Optimization of Machining Parameters of Photo Chemical Machining for Manufacturing Serpentine Micro Channels for Microreactors
3	Sridhar S.	07.02.15	Seismic Fragility Analysis of a Hot Cell Structure by Using Latin Hypercube Sampling Technique for Estimation of Fragility Parameters
4	S. Rajeswari	10.02.15	Evaluation of Hydrodynamic Suitability of N,N-Didodecyl N',N'-Di-Octyl Diglycolamide: A Potential Candidate for Minor Actinide Partitioning
5	S. Somasundaram	24.02.15	PBE Based Drop-Dynamics Simulation in an Unbaffled Stirred Tank Reactor
6	B. Thilak	24.02.15	Inertial Behavior of Fuel Particle Under Severe Accident Scenario in Pool Type Sodium Cooled Fast Reactor
7	Kinkar Mandal	24.02.15	Hydraulic and Mass Transfer Studies in a Single Stage 5- Inch Centrifugal Extractor

Titles of M.Phil. Theses for which results were notified during April 1, 2014 to March 31, 2015

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
1	V. Raman	30.10.14	Implementation of Number Field Sieve

Annex 6
Titles of D.M., M.Ch & M.D. Theses for which results were notified during April 1, 2014 to March 31, 2015

Titles of D.M., M.Ch & M.D. Theses for which results were notified during April 1, 2014 to March 31, 2015

Sr.No.	Title	Date of Notification of degree	Degree	Thesis Title
1	Dr. V.S. Pawan Kumar	18.07.14	MD-Anaesly.	Post operative analgesia following gynecological surgery – a retrospective comparison between epidural and IVPCA based analgesia.
2	Dr. Pooja Natarajan	18.07.14	MD-Anaesly.	Identification of optimally functional thoracic epidural analgesia – a prospective audit
3	Dr. Jain Surabhi Sushil	18.07.14	MD-Anaesly.	Audit of perioperative anaesthetic management of pancreaticoduodenectomy
4	Dr. Rohit Paliwal	18.07.14	MD-Anaesly.	Comparison of clinical utility of three different methods of ABG analysis in picking up hidden complex acid base disorders in critically ill patients.
5	Dr. Jain Mahendrakumar S.	18.07.14	MD-Anaesly.	Evaluation of CobraLA for airway management during general anaesthesia : Indian experience
6	Dr. Leena Chaudhari	18.07.14	MD-Anaesly.	Perioperative factors affecting free flap survival
7	Dr. Mapari Amol Pralhadrao	18.07.14	MD-Anaesly.	ReSOnS trial – Rectus Sheath block for postoperative analgesia in gynaec-onco surgical patients – a double blinded randomized controlled trial
8	Dr. Khandale Vijaykumar V.	18.07.14	MD-Anaesly.	Prospective Study comparing two different techniques of Proseal LMA Insertion
9	Dr. Tarwade Pritee Arun	18.07.14	MD-Anaesly.	Randomized trial to study the role of pre-intubation assessment of the airway using adult fibreoptic bronchoscope in achieving lung isolation using double lumen tubes and bronchial blockers.
10	Dr. Marudwar Prasanna P.	18.07.14	MD-Anaesly.	Referral of patients from Pre-anaesthetic checkup OPD for specialist consultation – an audit of current practice.

Sr.No.	Title	Date of Notification of degree	Degree	Thesis Title
11	Dr. Gavali Abhijit Shankarrao	18.07.14	MD-Anaesly.	Postoperative analgesia following abdominal surgery – an audit of clinical practice and patient satisfaction in a tertiary care cancer centre.
12	Dr. Patil Dipali Ravindra	18.07.14	MD- Immuno Hematology & Blood Transfusion	An Audit of Platelet Transfusions in a Tertiary Care Oncology Centre
13	Dr. Abhishek Chatterjee	18.07.14	MD-Rad.Thy.	Biological imaging before, during, and after simultaneous modulated accelerated radiation therapy in Head & Neck swuamous cell carcinoma (BIO-SMART)
14	Dr. Sayan Das	18.07.14	MD-Rad.Thy.	A Prospective Study to Evaluate the Incidence of Clinical Radiation Induced Pneumonitis in Lung Cancer Patients Treated with (Chemo) Radiotherapy
15	Dr. Manu Mathew	18.07.14	MD-Rad.Thy.	Dosimetric correlation of radiotherapy doses to neural ste, cel niche areas with outcome data in patients with newly diagnosed glioblastoma treated with conventional adjuvant therapy
16	Dr. Sangeeta Kakoti	18.07.14	MD-Rad.Thy.	Intensity modulated radiotherapy in sarcomas of Head and Neck and Pelvis and a Dosimetric Comparison with Proton Beam Therapy
17	Dr. Visariya Bhavin C.	18.07.14	MD-Rad.Thy.	Dosimetric comparison of conventional radiotherapy with two techniques of Tomotherapy viz. Helical Tomotherapy and Fixed beam Tomotherapy in Patients with synchronous bilateral breast cancer (SBBC) : A Pilot Study
18	Dr. David Bakirathrajan	18.07.14	MD-Pathlgy	Role of Transforming Growth Factor Beta in evaluating Tamoxifen resistance in Harmone Receptor Positive breast Cancer–A Retrospective Case Control Study
19	Dr. Verma Anuj	18.07.14	MD-Pathlgy.	Exploring CD137 and CD137L in Mediastinal Lymphoma – Attempt at segregating the Black (PMBCL) and White (CHL) from the Gray Zone

Sr.No.	Title	Date of Notification of degree	Degree	Thesis Title
20	Dr. Nagaraj T.S.	18.07.14	MD-Pathlgy.	Testing of MYCN GENE amplification status in patients with neuroblastoma and correlation with histomorphological features
21	Dr. Pramod N. Biradar	18.07.14	MD-Pathlgy.	Feasibilty of Application and Sub typing of Lung Adenocarcinoma as per the Proposed IASLC 2011 Multidisciplinary Classification of Lung Adenocarcinoma
22	Dr. Correia Sabina	18.07.14	MD-Pathlgy.	Immunohistochemical expression of Epidermal Growth Factor Receptor (EGFR) in Non-Small Cell Lung Carcinoma (NSCLC) and its clinical significance
23	Dr. Pradhan Anuja	18.07.14	MD-Pathlgy.	Descriptive Report on Spectrum of Cases Seen in Gynaecological Cancers. A Study of Gynaecological Pathology Reports Diagnosed in the Department of Pathology, in One Year (2011)
24	Dr. Modkharkar Sushil	18.07.14	MD-Pathlgy.	An Audit of One Year Surgical Pathology Reports of Nodal and Extranodal Hematolymphoid Neoplasms
25	Dr. Badanale Renuka	18.07.14	MD-Pathlgy.	Audit of Biopsies and resections from trunk and Extemity – based Soft Tissue Tumours
26	Dr. Mistry Kunal Arvindbhai	18.07.14	MD-Radio-Diagnosis	Mammographic changes in breast cancers post Neo adjuvant Chemotherapy
27	Dr. Rajeshkumar Das	18.07.14	MD-Radio-Diagnosis	Prospective study of the mammographic features of operable breast carcinoma
28	Dr. Udare Amar Ramesh	18.07.14	MD-Radio-Diagnosis	Pre and Post-operative tumour estimation of Glimas using Magnetic Resonance Imaging
29	Dr. Pawar Dilip Jambuwant	18.07.14	MD-Radio-Diagnosis	Correlation of CT based Recist response post Neo Adjuvant chemotherapy with Histopathological response at post-operative specimens in patients eith Esophageal Cancer
30	Dr. Tamhankar Anup Sunil	18.07.14	MCh.- Surg. Oncology	Impact of age as an independent prognostic factor for lymph node metastasis and survival in breast cancer.

31	Dr. Ashish Gulia	18.07.14	MCh.- Surg. Oncology	Oncological outcome of extremity synovial sarcomas treated with multimodality management.
32	Dr. Vallam Karthik Chandra	18.07.14	MCh.- Surg. Oncology	A retrospective analysis of salvage neck dissections after definitive radiation / chemoradiation in head & neck squamous cell cancers.
33	Tathe Nitin Achyutrao	18.07.14	MCh.- Surg. Oncology.	Evaluation of appropriateness of surgery in patients with locally advanced adenocarcinoma rectum with borderline resectability post nactrt.
34	Dr. Caleb Harris	18.07.14	MCh.- Surg. Oncology.	The impact of optic nerve resection length on survival in retinoblastoma.
35	Dr. Bhandare Manish Suresh	18.07.14	MCh.- Surg. Oncology.	Retrospective audit – Treatment of Non Metastatic Primary Sacral Tumors.
36	Dr.Ashwin Luis Desouza	18.07.14	MCh.- Surg. Oncology	A comparison between laparoscopic and open surgery for colorectal cancer.
37	Dr. Nag Snita Shankar Kumar	18.07.14	MCh.- Surg. Oncology.	Role of retroperitoneal lymph node dissection in intermediate and high risk patients.
38	Dr Vishwas Pai D.	18.07.14	MCh.- Surg. Oncology	Impact of definitive surgery on health related quality of life in patients with resectable esophageal cancer.
39	Dr. K. Girish Kumar	18.07.14	MCh.- Surg. Oncology	Prospective evaluation of subject`s understanding of informed consent about their planned surgery and adequacy of consent in cancer surgery.
40	Dr. Shubham Jain	18.07.14	MCh.- Surg. Oncology	A retrospective audit to study the effect of Tamoxifen on mammographic breast density in breast cancer patients.
41	Dr. Eugene George Rent	18.07.14	MCh.- Surg. Oncology	Correlation of PET scan findings with histopathology and survival in head and neck malignancies.
42	Dr. Guruchannabasavaiah B.	18.07.14	MCh.- Surg. Oncology	To study expenditure on major Gastro-intestinal cancer surgery in Tata Memorial Centre.
43	Dr. Tanushree Jain	18.07.14	MCh.- Gynec Oncology	Retrospective audit of a prospectively maintained database of Total Laparoscopic Radical Hysterectomy (TLRH) for early-stage cervical carcinoma FIGO Stages IA2-IB2.

Sr.No.	Title	Date of Notification of degree	Degree	Thesis Title
44	Dr. Deepa Susan Roy Philip	18.07.14	DM-M.Ocly.	A retrospective analysis of clinical characteristics, treatment and outcome of children with Anaplastic Large Cell Lymphoma treated at Tata Memorial Centre from 1997-2011.
45	Santhosh Kumar D.	18.07.14	DM-M.Ocly.	Retrospective analysis of outcomes of patients with relapsed, refractory and metastatic sarcomas who have received metronomic chemotherapy.
46	Dr. Alok Gupta	18.07.14	DM-M.Ocly.	Anthracycline Induced Cardiotoxicity in Osteogenic Sarcoma Patients: A case control study.
47	Dr. (Ms.) Nidhi Tandon	18.07.14	DM-M.Ocly.	Baseline high resolution CT scan thorax for detecting repiratory infection in patients with acute myeloid leukemia at presentation.
48	Dr. Avinash Vijaykumar Pandey	18.07.14	DM-M.Ocly.	Outcomes of multiple myeloma in the era of novel agents: A retrospective study from tertiary cancer centre.
49	Dr. Aseem Kumar Samar	18.07.14	DM-M.Ocly.	Prognostic and predictive factors for use of palliative chemotherapy in advanced stage esophageal / gastroesophageal junction cancer.
50	Dr. (Ms.) Nishitha Shetty	18.07.14	DM-M.Ocly.	The dynamics of circulating nucleosomes following adjuvant neoadjuvant or palliative chemotherapy for early breast cancer (EBC), locally advanced breast cancer (LABC) and metastatic breast cancer (MBC).
51	Dr. Ashish Singh	18.07.14	DM-M.Ocly.	A retrospective analysis of clinical characteristics, treatment and outcome of patients with locally advanced or metastatic gall bladder cancer treated at Tata Memorial Centre, Mumbai from January 2012 to Oct. 2013.
52	Dr. Bharat Chauhan	18.07.14	DM-M.Ocly.	Diagnostic utility of 18F FDG-PET/CT in the detection of bone marrow disease in Hodgkin`s lymphoma and their prognostic significance. A retrospective study.

53	Dr. Sachin Bharatbhai Punatar	18.07.14	DM-M.Ocly.	An open labeled randomized trail comparing oral iron versus intravenous iron for the treatment of cancer induced anemia.
54	Dr. Sheth Vipul Sharad	18.07.14	DM-M.Ocly.	Outcomes of Acute Myeloid Leukemia with translocation t (8,21) : A retrospective study from tertiary cancer centre.
55	Garud Aniruddha Pandharinath	19.01.15	MD-Pathlgy.	To evaluate correlation of the histomorphological variables of primary tumour with presence of ECS in the nodal metastasis
56	Kaushal Kishor Yadav	19.01.15	MCh.- S.Ocly.	Evaluation of the prevalence of functional problems after oral cavity malignancy surgery using PSS HN(Performance Status Scale for Head and Neck) Scale.
57	Srivastsa H.G.	19.01.15	MCh.- S.Ocly.	Analysis of patterns of failure in lung cancer (NSCLC) patients undergoing radical resection- A retrospective study.
58	Mathankar Manish Jagdishrao	19.01.15	MD-Rad.Thy.	Retrospective audit – Treatment of Non Metastatic Primary Sacral Tumors.
59	Chandre Mukesh Bhavsing	19.01.15	MD-Rad.Thy.	A Retrospective study of post cricoid, upper cervical and thoracic oesophageal cancer treated with radical non surgical treatments in TMH

i

प्रशिक्षण विद्यालय परिसर के आंतरिक आंगन का दृश्य

A view of inner courtyard of Training School Complex

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