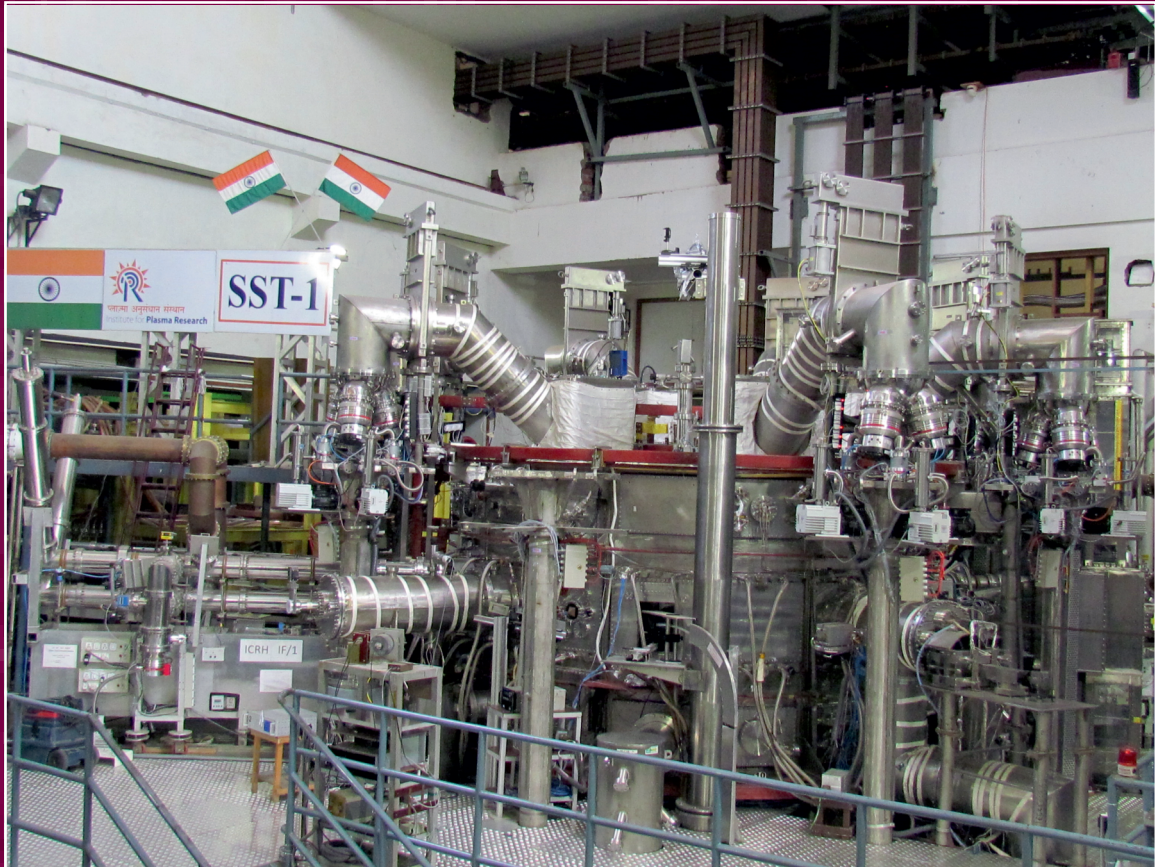


होमी भाभा राष्ट्रीय संस्थान Homi Bhabha National Institute



Academic Report 2013 - 2014



Training School Complex
Anushaktinagar, Mumbai 400 094

Constituent Institutions (CIs) of HBNI

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.

Front cover page photograph : Steady State Super-conducting Tokamak (SST-1) at the Institute for Plasma Research (IPR) where the first plasma was achieved in June 2013.

Homi Bhabha National Institute

Academic Report 2013-2014



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From the Director

Higher education in India is going through unprecedented expansion. In spite of impressive growth in the recent years, Gross Enrolment Ratio (GER) for the age group 18-23 is only 19%¹. The ongoing 12th Five Year Plan envisages a quantum jump in the GER². There is a concern about the fact that universities in India do not find a place amongst the top global universities. To address all issues related to higher education, the Government has launched ‘Rashtriya Uchchatar Shiksha Abhiyan’ (RUSA)³, a campaign for



To improve quality of higher education, among other aspects, the RUSA recognizes the importance of research and research universities. It says, “Research universities stand at the centre of the 21st century global knowledge economy and serve as flagships for higher education worldwide.” Philip G. Altbach defines research universities as “academic institutions committed to the creation and dissemination of knowledge, in a range of disciplines and fields, and featuring the appropriate laboratories, libraries, and other infrastructures that permit teaching and research at the highest possible level.”⁴ While a vast majority of post-secondary institutions focuses on under-graduate education, the focus in a research university is research and research based degrees.

Simultaneous with its expansion, higher education is coming closer to work places. This is influencing both: the way higher education is designed in terms of curriculum and topics of research, and the way work places go about their work. Constraints imposed by rising costs of inputs due to depleting resources and concerns about sustainability of resources and environment are propelling industries to work closely with researchers from universities. The academics in the universities are looking up to industry for funding research and are tailoring their research to meet industry requirements.

¹ Report on All India Survey on Higher Education (2010-11), released in 2013.

² University Grants Commission, “Inclusive and Qualitative Expansion of Higher Education: 12th Five Year Plan, 2012-17.

³ http://www.mhrd.gov.in/sites/upload_files/mhrd/files/RUSA_final090913.pdf

⁴ Philip G Altbach, “Advancing the national and global knowledge economy: the role of research universities in developing countries”, Studies in Higher Education, 2013, Vol 38, No 3, 316-330.



Several academic programmes in universities and institutes have been designed to tailor to the requirements of work places.

Focusing on research, one notes that the national research framework in India has a particular structure. A major fraction of the research funded by the Central Government is conducted in the national laboratories and a majority of them belong to the Department of Atomic Energy (DAE), the Department of Space (DOS), the Defense Research and Development Organization (DRDO) and the Council of Scientific and Industrial Research (CSIR). Realizing the importance of university functions and also the importance of efficiently discharging those function, all these agencies have to some extent internalized such functions. The DAE has two deemed universities under its fold viz., Tata Institute of Fundamental Research (TIFR) accredited in May 2002 and Homi Bhabha National Institute (HBNI) accredited in June 2005. The DOS has the Indian Institute of Space Science and Technology (IISST) set up in 2007 and accredited as a deemed to be university in July 2008. The DRDO has Defense Institute of Armament Technology, DIAT Which was accredited as a deemed to be university in September 1999, and the CSIR has set up the Academy for Scientific and Innovative Research AcSIR under an Act of Parliament notified in 2012 Apart from (IISST) and DIAT, focus in other universities viz., HBNI, TIFR and AcSIR is on post-graduate education and research. This development brings in a new concept of a research university.

Speaking about HBNI, it is a research university. Its faculty, which is based in its Constituent Institutions, is primarily engaged in research. It is rigorously meritocratic in hiring and promotion of faculty, admissions and progression of students and in everything it does. Since its constituent institutions had been engaged in research prior to its setting up, it has been able to hit the ground running.

This annual report gives a brief account of the activities during 2013-14 and also tells all about the Institute at a glance. Its output of doctoral theses and other post-graduate degrees is indeed impressive and continues to steadily grow.



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 interdisciplinary 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	Director 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.	L.M. Gantayet	1950	2005	BARC
13.	T. Jayakumar	1955	2005	IGCAR
14.	B.B.Biswas**	1948	2006	BARC
15.	Manjit Singh	1950	2006	BARC
16.	S. Venugopal	1955	2006	IGCAR
17.	A.K.Bhaduri	1959	2007	IGCAR
18.	G K Dey	1957	2008	BARC
19.	K. Velusamy	1959	2008	IGCAR
20.	R.R.S. Yadav	1952	2008	BARC
21.	U. Kamachi Mudali	1960	2009	IGCAR
22.	P.K. Wattal	1951	2010	BARC
23.	K.K. Jayarajan	1962	2011	BARC
24.	R. Natarajan	1953	2011	IGCAR
25.	K.K. Vaze	1950	2011	BARC
26.	R.K. Singh	1953	2012	BARC
27.	A.K. Sinha	1956	2012	BARC
28.	S. Chaturvedi	1962	2013	BARC
29.	C.K. Pithawa	1951	2013	BARC
30.	S.B. Roy	1956	2013	BARC

* Homi Bhabha Chair

** Raja Ramanna Fellow (RRF)

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

	Name	Year of Birth	Year of Election	CI
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

*Homi Bhabha Chair, **RRF, ***DST Professor, ****S. Chandrasekhar Chair



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	1952	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. Chandrasekar	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

*Homi Bhabha Chair, **RRF, ***DST Professor, ****S. Chandrasekhar Chair

**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.	Dilip 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

*Homi Bhabha Chair, **RRF, ***DST Professor, ****S. Chandrasekhar Chair

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.	Swapam K. Ghosh	1949	2010	BARC

*Homi Bhabha Chair, **RRF

7. Fellow of World Academy of Art and Science

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

*Homi Bhabha Chair

**8. Recipient of National Civilian Awards**

	Name	Year of Birth	Year of Award	CI
Padma Vibhushan				
1.	Anil Kakodkar*	1943	2009	BARC
Padma Bhushan				
2.	Anil Kakodkar	1943	1999	BARC
3.	Ashoke Sen	1956	2013	HRI
4.	J B Joshi	1949	2014	HBNI
Padma Shri				
5.	P K Kaw**	1948	1985	IPR
6.	Anil Kakodkar	1943	1998	BARC
7.	Ashoke Sen	1956	2001	HRI
8.	Srikumar. Banerjee*	1946	2005	BARC
9.	R. Balasubramanian	1951	2006	IMSc
10.	R. A. Badwe	1956	2013	TMC
11.	S P Kale	1954	2013	BARC
12.	R. B. Grover*	1949	2014	HBNI
13.	Sekhar Basu	1952	2014	BARC

*Homi Bhabha Chair, ** DST Professor



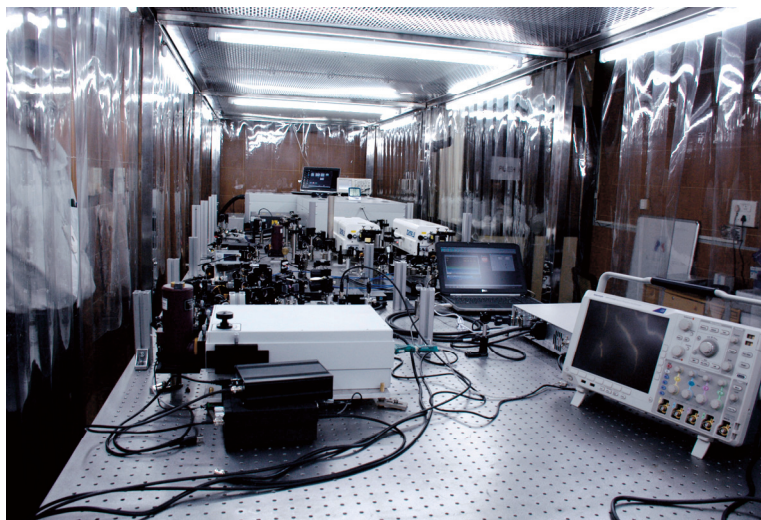
News from Constituent Institutions (*in brief, details available at respective websites*).

Bhabha Atomic Research Centre (www.barc.gov.in)

Interaction of radiation with matter: Effect of both high energy radiation (electron beam and gamma-radiation as well as lower energy photons (X-ray – UV-Visible-IR-THz) on molecules and materials is investigated with an aim to a) understand the processes responsible for radiation damage and remedy, prescription of synthesis and usage of new and better materials, b) exploring the possibilities of use of radiation in agriculture, biology and medicine, c) to understand the light or laser induced molecular processes related to the laser isotope enrichment processes, d) harvest solar energy, and e) search for advanced photonic and biological materials in the form of supramolecules and nanoaggregates.

Fundamental studies of radiation chemistry of water under nuclear reactor conditions, antioxidants and radio protectors, radiation polymerization, development of polymer-extractantcomposites

for extraction of radionuclides & toxic metals are also taken up. Radiation stability of extractants and polymericcomposite materials, utilization of radiation and photochemical processes for hydrogen generation, treatment of selected waste from nuclear & other industries, dielectric barrier discharge chemistryand free radical chemistry at surface and interface.Pulse Radiolysis is being used routinely for studying the kinetics of high energy electron beam (low LET radiation) induced chemical reactions in aqueous solutions, organic liquids, solids and polymeric systems. Development of a new pulse radiolysis system based on indigenously developed laser driven picosecond electron accelerator, has been taken up to improve the time resolution from nano to picosecond.



2D IR spectrometer

Chemical reaction dynamics: In the field of Dynamics and Kinetics of chemical reactions in the gas phase BARC is engaged in investigations of photo-dissociation dynamics of polyatomic molecules Using LIF and REMPI techniques, kinetics of atmospherically important reactions, photochemistry at surfaces and interfaces using sumFrequency generation (SFG) technique. In

solution phase, interfacial electron transfer dynamics relevant to solar energy conversion, excited state relaxation dynamics of intra and intermolecular charge transfer, proton transfer and conformational relaxation dynamics, solvation and rotational dynamics, Inter and Intra-molecular hydrogen bond dynamics and coherent control of chemical reactions are being investigated using indigenously developed fast and ultrafast spectroscopic techniques.

Studies on diffusion of hydrogen and deuterium in Zr-2.5% Nb alloy: For life time management

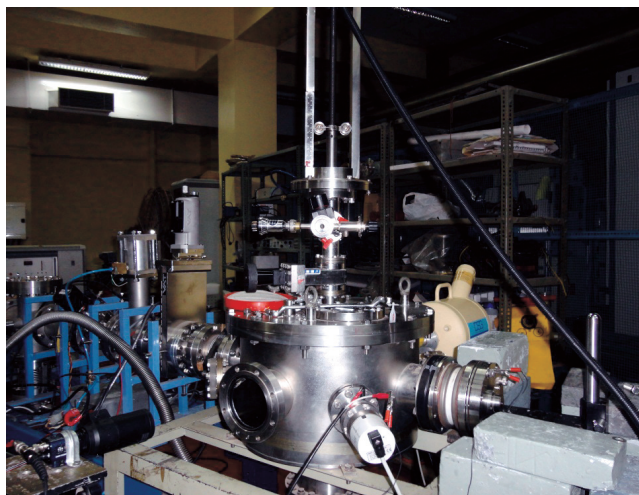


Photograph of the HVE-QMS system, at RACD, BARC

of operating coolant channels, hydrogen/deuterium is being determined at regular time intervals for the last two decades employing hot vacuum extraction cum quadrupole mass spectrometer (HVE-QMS). With a view to understand the trend of H/D concentrations in the sliver samples, diffusion studies of hydrogen and deuterium in Zr-2.5% Nb alloy were carried out at different temperatures. The activation energy of deuterium diffusion in Zr-2.5% Nb was found to be higher than that of hydrogen.

Determination of boron in thick samples by PIGE: A method has been standardized to

determine boron content in borated paraffin wax samples non-destructively. The method employs proton induced gamma ray emission (PIGE) using proton beam from Folded tandem Ion Accelerator (FOTIA) and Trombay. Owing to the large thickness of the samples, the proton beam is stopped in the samples and hence the beam current cannot be measured. This makes the quantification difficult unless a suitable monitor is used. In the present work the sample was wrapped with a thin (2 mg/cm^2) aluminium foil and the gamma rays emitted from the $^{27}\text{Al}(p,p'\gamma)^{27}\text{Al}$ reaction were used to normalize the beam current.



Photograph of the PIGE system at FOTIA, BARC



Life Sciences activities : BARC has a vibrant program of basic and applied research in life sciences encompassing a wide spectrum of studies. The flagship programs of the institute include, (a) use of radiations and radioisotopes in contemporary thrust areas of research, of excellence and relevance to the DAE programs and of national interest (b) long-term studies on effects of high background natural radiations on human populations living in coastal areas of Kerala (c) radiation-induced mutagenesis for crop improvement (c) use of radiations and other technologies for disinfection, hygienisation and preservation of food, improvement of nutritional quality and extension of shelf life, to enhance food security (d) development of radiopharmaceuticals and equipments for diagnosis and therapy of a variety of human diseases, and (e) development of appropriate technologies to strengthen the aforesaid programs and for application in environmental clean-up.

Biology of stress and adaptive responses of microbes and plants is one of the strong points of basic and applied research at BARC. Genomic, proteomic and bioinformatic approaches have been used to discover new genes, their functions and regulation, and to assess their role in the extreme radiation resistance of *Deinococcus radiodurans* and radiation and agricultural stress tolerance of nitrogen-fixing cyanobacteria such as *Anabaena* strains. Recombinant DNA technology has been very effectively used to genetically engineer microbes for eco-friendly biotechnological applications as nitrogen biofertilisers in stressful environments, as biosensors of agronomically important pesticides or as biopesticides. Novel organisms have been discovered with unique abilities to sequester uranium from 3 ppb concentrations found in seawater or to degrade and utilize the major nuclear solvent tributyl phosphate (TBP). Radioresistant recombinant strains of *Deinococcus* have been constructed to bioprecipitate uranium over a wide range of concentrations and pH from high radiation environments.

Effects of high background natural radiation that prevails in monazite sands of Kerala are under investigation for last 4 decades in BARC. A survey of 1.5 lakh newborns has been carried out in recent years to reveal no significant effects attributable to radiation on congenital malformations, cytogenetic defects, Down's syndrome, DNA damage and repair, mutation rate etc. In parallel, radiation effects are being investigated in cell lines and animal models to assess bystander effects, damage caused by metals like uranium/thorium and methods of their decorporation from tissues, and molecular markers of carcinogenesis and metastasis. Heavy ion irradiation and alpha particle irradiation effects are also under investigation. Attempts are also on to develop natural products as immunomodulators and radioprotectors and as effective regulators of signal transduction pathways to alleviate/enhance radiotoxicity to normal/tumor cells respectively.

Radiation-induced mutagenesis for crop improvement is one of the very successful programs in Life Sciences at BARC. To date 42 new improved varieties of different crops have been



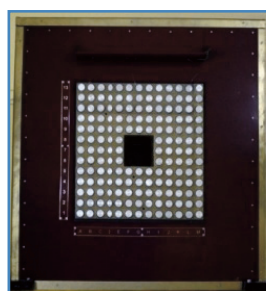
developed by BARC and released by ICAR and State Agricultural Universities for cultivation in various states of India. While oilseed varieties, such as groundnut, mustard, soybean, and pulses, such as mungbean, urdbean and pigeonpea, are the more successful programs, varieties have also been developed in crops such as rice, jute, sunflower and cowpea. Gamma irradiation and electron beam based food irradiation programs have been designed by BARC for a variety of purposes, such as sprouting inhibition in onions and potatoes, disinfestations of grains and resins, shelf-life extension of several ready-to-cook and ready-to-eat items including meat products, and decontamination of spices. Applications have been developed for quarantine purpose for export of mangoes or foods for disaster management or for immune-compromised patients etc. BARC also designs and fabricates equipments required for such programs and makes them available to other users through technology transfer programs.

Development of radiopharmaceuticals, including production of ^{18}F -FDG using medical cyclotron at BARC, and establishment of state of art imaging technologies using PET-CT machines have strengthened disease diagnostic capabilities at BARC and triggered substantial research on diagnosis of tuberculosis and other infectious disease, apart from variety of cancers and neural disorders etc. Design and fabrication of indigenous teletherapy machines (Bhabhatron) has greatly benefitted patients awaiting radiotherapy. Nisargaruna biotechnology, for conversion of organic waste to methane and to electricity, has not only proven to be technologically robust but has also been extremely popular as manifested by setting up of over 160 such plants all over the country in last 6-7 years. The solar dryers for food preservation, biosensors for pesticides and metal removal biotechnologies developed in last 2-3 years are likely to find field applications in near future. All the aforesaid research and development activities in Life Sciences have been published in high impact, peer-reviewed international journals and have been recognized in the form of very prestigious awards, fellowships and other such honors.

The Physics Group in BARC continues to pursue R & D programmes in Physics which are at the cutting edge of research and also relevant to the DAE mandate. There is an active basic research programme which spans a large range of energy, time and length scales and includes a comprehensive study of matter at extremes. Interfaced with these programs, the Group also pursues the indigenous development of technologies covering precision instrumentation, particle accelerator, synchrotron and neutron beam lines at Dhruva and a high energy gamma ray telescope. Some of the highlights achieved in this period are described in this executive summary.

In the area of nuclear physics a precise measurement of the radioactive transition in ^8Be has been carried out and the new result motivates a calculation that combines state of art *ab-initio* structure calculations with reaction models of the alpha-alpha collision process. The role of

cluster structure of ${}^7\text{Li}$ on the dynamics of fragment capture was studied through exclusive measurements of prompt γ -rays from heavy-residues in coincidence with light charged particles in the ${}^7\text{Li} + {}^{198}\text{Pt}$ system. The indigenously designed and developed 400 keV, 4 vane Radio Frequency Quadrupole (RFQ) was commissioned in pulsed mode. Under high pressure physics domain the studies on reduced graphene oxide, theoretical as well as experimental studies on glycine lithium sulphate have generated several novel findings. In this context, the importance of onsite Coulomb interactions between the 5f electrons in the determination of the various ground state and high pressure properties of actinides has been investigated. Surface Enhanced Infrared Absorption (**SEIRA**) has been developed for the study of organic and biologically important molecules. For laser-matter interaction studies a high resolution and high dispersion Thomson parabola spectrometer (TPS) with time-of-flight unit was developed for characterization of ions produced in laser generated plasma, and also to calculate the hydrodynamic parameters. The oxalate and phenanthroline ligands based 1-D single chain molecular magnets have been demonstrated.



Subcritical core

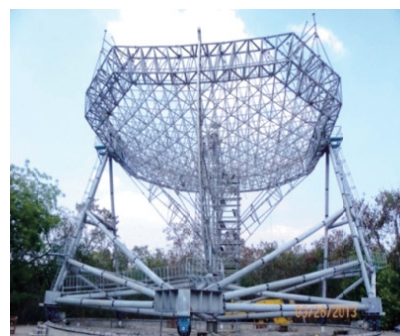
In the areas of developing advanced technology for frontier physics researches several state-of-the-art facilities have been established. A subcritical assembly driven by a D-D / D-T neutron generator has been successfully developed and commissioned. The development of



Purnima Neutron Generator

such a zero power facility will enable study of various physics parameters related to neutronics, reactor physics and dynamic characteristics of Accelerator Driven System (ADS). Active neutron interrogation technique for detection of fissile material in bulk material using pulsed neutron generator has been developed in the Group. Recently thermoelectric material CuCrSe_2 is investigated with figure of merit (ZT) ~ 1 at 773 K. The Group has indigenously developed inductively coupled plasma Mass Spectrometer (ICPMS) system.

The TACTIC telescope at Mt. Abu was deployed for TeV (10^{12} eV) gamma-ray observations of extragalactic objects. The 240 KWp solar power plant required for the MACE telescope has been installed and commissioned at Hanle. A 9-meter long cylindrical multi-cathode magnetron sputtering system for fabrication of mirrors and super mirrors for X-ray and neutron applications has been successfully installed and commissioned. A hybrid detector telescope has been developed for the simultaneous



Trial assembly of the MACE telescope in progress at ECIL, Hyderabad



detection of a wide range of charged particles. An indigenously developed Multi-Cathode Source of Negative Ions by Cesium Sputtering source system is commissioned at Pelletron-Linac accelerator facility successfully, delivering negative ion beams across the periodic table. The Group provided engineering support in development & commissioning of an indigenous desktop Alpha Particle Irradiator for *in vitro* radio biological studies for radiation risk assessment under various radiation exposure conditions. A time-domain based low-coherence fibre-optic interferometer has been indigenously developed for depth-resolved tomography imaging of scattering samples for material science research. A 2-D Position Sensitive Detector (PSD) for neutron beam imaging is developed.

In the domain synchrotron radiation and its utilization for science researches, several noteworthy achievements have been made. The protein crystallography (PX) beamline has been augmented with an auxiliary biochemical laboratory and cold rooms. X-ray Absorption Fine Structure Spectroscopy (XAFS) at BL-08 and BL-09 beamline has been utilized for Ayurvedic Drugs qualification experiments. The HRVUV (high resolution vacuum ultraviolet) beamline at Indus-1 SRS was utilized for characterization of the specialized gas cells used in the Lyman Alpha Photometer (LAP) payload on the Mars Orbiter Mission launched by ISRO in November 2013.

Under international research collaboration programs, the Group is providing several critical modules and sub-modules to ILL, France. The Group has also contributed in the Resistive Plate Chamber (RPC) upgrade project for the Compact Muon Solenoid (CMS) experiment, CERN, Geneva, Switzerland.

Engineering sciences : BARC have been pursuing the research and development programmes in the frontal areas of engineering science and technology. Several spin off technologies have been developed having direct societal relevance and were transferred to the public domain for further commercial exploration thus translating the laboratory research outcomes for the benefit of common man. A brief narration of some of the accomplishments made by engineering sciences during the year 2013-2014 is presented below.

- BARC has demonstrated its capability in making industry ready 80 kV, 12 kW Electron beam welding (EBW) machine.
- BARC has developed inductively coupled plasma mass spectrometer (ICPMS) and transferred the technology to M/S Elico, Hyderabad.
- Completely bio-degradable polymers based on polycaprolactone and partially bio-degradable linear low density polyethylene using radiation processed thermoplastic starch was developed.



- BARC has developed a new supercomputer, “ANUPAM-Aggra” using parallel processing technology. This supercomputer is the largest and fastest in the ANUPAM series of supercomputers.
- Online Thoron Mitigation System (**OTMS**) has been indigenously developed to control the thoron (^{220}Rn) gas emission into environment through stack of upcoming Power Reactor Thorium Reprocessing Facility (PRTRF) based on charcoal adsorption technique.
- BARC has successfully completed full scale 3-D MHD numerical simulation of the Indian Test Blanket Module (TBM) of International Thermo nuclear Experimental Reactor (ITER) project.
- A Tele Distress Alarm Device, named **Nirbhaya**, has been developed and the technology has been transferred to ECIL for mass production.
- A 12-Channel battery operated portable ECG Machine is developed. **DORAbot** (Detection Of Radiological Activity using a Robot) is a tracked mobile robot with cameras and radiation sensor packs to scout radioactive areas in and around nuclear installations in the event of a radiological emergency was developed.

Indira Gandhi Centre for Atomic Research (www.igcar.gov.in)

Fast Breeder Test Reactor (FBTR)

- The Fast Breeder Test Reactor (FBTR) acquired license to operate until June 2018.
- A comprehensive report has been prepared after the completion of feasibility study of locating 500MWt Metal fuel Demonstration Fast Reactor (MDFR) at Kalpakkam.

Kamini Reactor

- Kamini Reactor was operated at different power levels for neutron radiography of pyro devices from Vikram Sarabhai Space Centre and tungsten rods from Defence Research Development Organisation.

Prototype Fast Breeder Reactor (PFBR)

- Construction of 500MWe Prototype Fast Breeder Reactor is nearing completion. Despite technological challenges of first of the kind, the sodium cooled reactor has achieved an overall physical progress of 97.61%. (Figure Enclosed)

Fast Reactor Fuel Cycle Facility (FRFCF)

- Financial approval of FRFCF project was received and construction work has started.

Technology Development



Full scale model of passive sodium fire mitigation for

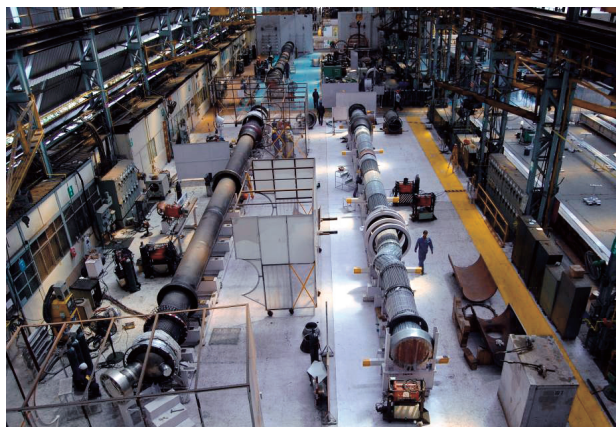
- A sodium fire facility was commissioned to study the atmospheric dispersion of sodium aerosol in the event of sodium fire. (Figures Enclosed)
- Thickness of primary pump bellows of PFBR was optimized for various aspects related to

pump performance and the bellows were manufactured by the local industries with complete technical support from IGCAR.

- Adjacent tube wastage experiments on 9 Cr-1 Mo steam generator tube specimens have been completed. These specimens were supplied by CEA, France as part of collaborative agreement. The experiment results will be utilized for validating the code named PROPANA.



Prototype Fast Breeder Reactor (PFBR)



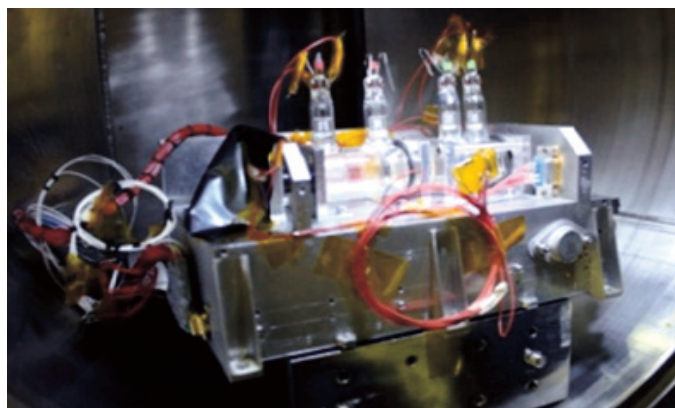
Modified 9Cr-1Mo steel with improved properties as future material for steam generators

A state of the art high-temperature (up to 1450^oC) split furnace, capable of controlled heating and cooling, has been developed and integrated with the indigenously developed high strain rate compression testing machine.

- India-specific RAFM (INRAFM) steel has been developed for
- Fusion reactors. The development is based on the detailed investigation of physical, micro-structural and mechanical properties including impact, tensile low cycle fatigue and creep on four heats of RAFM steel having varying tungsten and tantalum contents.

Raja Ramanna Centre for Advanced Technology (www.rrcat.gov.in)

The Indus-1 and Indus-2 synchrotron beamlines at RRCAT are being used by a large number of researchers from several universities, IITs, IISERs, national institutes like PRL, IISc, BARC, TIFR,

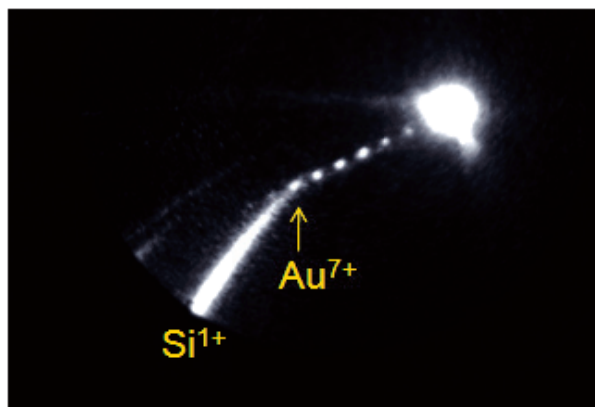


Gas-cell payload for the Mangalyaan

IGCAR, and UGC-DAE-CSR. Various subsystems of Indus-2 synchrotron have been upgraded, viz. microtron injector, RF power system, booster synchrotron, ultrahigh vacuum cooling system, and magnet power supplies. The output power of the solid state radio-frequency amplifiers has been increased to 225 kW. A bunch-by-bunch feedback system has also been installed for controlling the transverse coupled

bunch instabilities. As a result, the Indus-2 current has been increased to more than 180 mA at 2.5 GeV energy. The existing x-ray micro-focus beamline in Indus-2 has been upgraded with the total external reflection x-ray fluorescence facility. The x-ray lithography beamline has been used for fabrication of compound x-ray refractive lenses. An infra-red beamline has been installed on Indus-1, thus taking the total number of beamlines on Indus-1 to six. These beamlines have been used for a variety of experiments ranging from studies of multilayer x-ray optics to calibration of Lyman-alpha photometer gas-cell required for Mangalyaan mission.

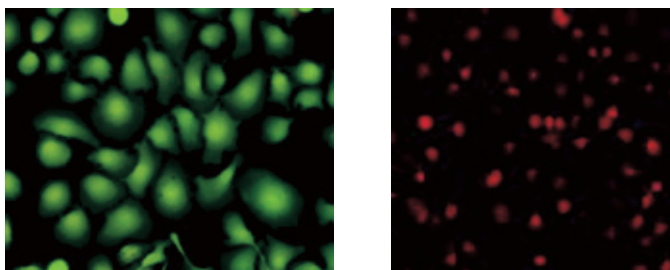
Experiments on ion acceleration carried out using a 10 TW Ti:sapphire laser focussed to an intensity of $\sim 2 \times 10^{18}$ W/cm² showed highly repeatable, mono-energetic, multi-species gold ion emission from gold-carbon co-sputtered nano-composite samples on silicon substrate.



Quasi-mono-energetic gold ions of different charge states (Au^{+1} to Au^{+7}) observed in ultra-intense laser plasma interaction

An optical parametric chirped pulse amplification based Nd:glass laser system of 40 TW peak power has been developed. It provides 24 J laser pulses of 600 fs duration. It is the highest peak power laser built in the country. A prototype model of 20 kW peak power (1 kW average power) industrial Nd:YAG laser with dual-port fiber optic beam delivery has been developed. The laser will find applications in the decommissioning of RCC walls of power reactors as well as in deep penetration welding.

An x-ray activable copper-iodide complex of chlorin p6 (Cp6-COP) has been synthesized for photo-dynamic therapy (PDT) of cancer and potential use in deep tumor treatment using x-rays (Fig. 3). The formation of the complex has been confirmed by visible, infrared, ESR and XRF spectroscopy.



Cancer cells stained with cancer cells death marker: (a) Live cancer cells in un-treated sample (green); (b) Cell death after PDT (red).

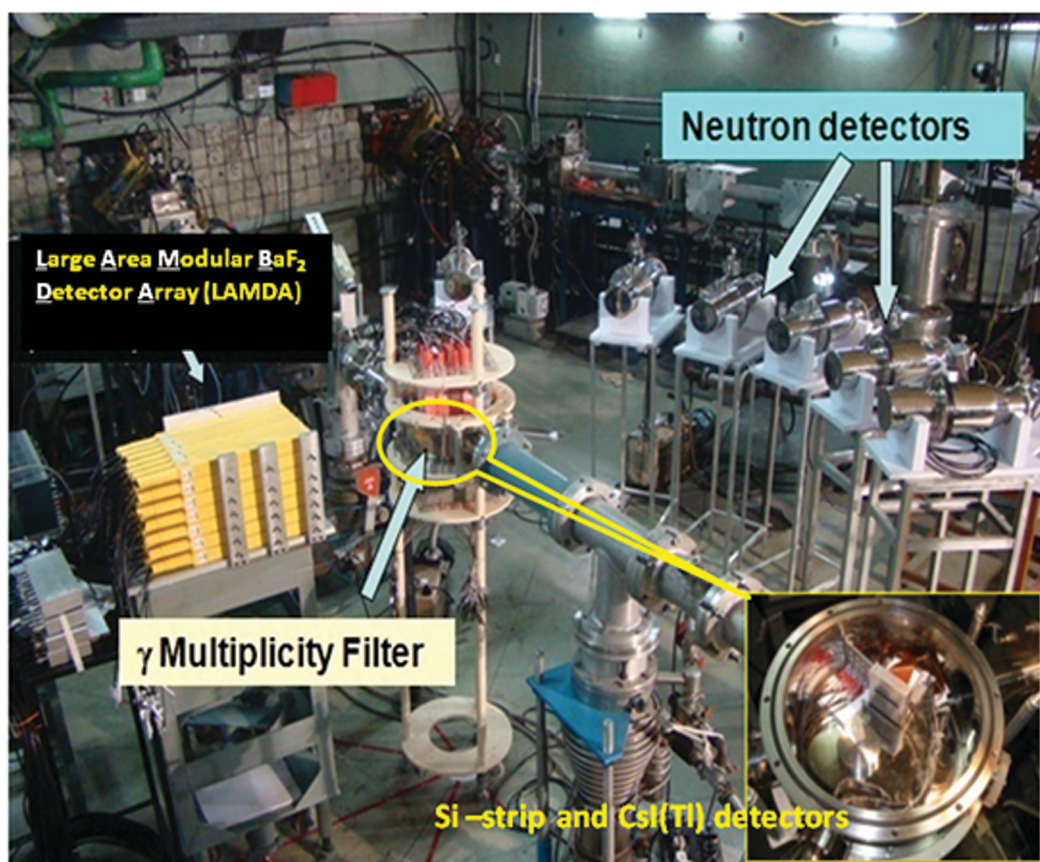
The electrical and magnetic properties of the superconducting Ti-V alloys have been studied as materials alternative to niobium in a high neutron-irradiation environment. The studies revealed important technological aspects related to the dependence of critical current on the presence of different metallurgical phases and defect structures.

Variable Energy Cyclotron Centre (www.vecc.gov.in)

Decay of Hoyle state: The Hoyle state, second O_2^+ resonant excited state of ^{12}C at excitation energy of 7.654 MeV, plays an important role to understand a variety of problems of nuclear astrophysics such as elemental abundance as well as the stellar nucleosynthesis process as a whole. From the nuclear structure point of view too, there are many unanswered questions regarding the configuration of this state; experimentally, it was found from inelastic scattering that this state has an abnormally larger radius compared to the ground state of ^{12}C ; theoretically, it has been conjectured as the lowest state corresponding to a different configuration (gaslike structure, member of a β band of the three- α molecule-like structure, or Bose-Einstein condensate-like structure), and even the possibility of a very unusual linear chainlike structure of three α particles has also not been ruled out. The standard shell-model approaches, even the advanced no-core calculations, failed to reproduce the state; however, recent *ab-initio* calculations using chiral effective field theory and Monte Carlo latticesimulation has been able to find a resonance in ^{12}C having the characteristics of the Hoyle state.

In nucleosynthesis reaction rate calculations, it is implicitly assumed that the decay of the Hoyle state proceeds exclusively via a sequential two-step process, i.e., via the ground state of 8Be . However, it is likely that the above-mentioned unusual structure of this state may modify the decay mode of ^{12}C , thereby affecting the reaction rate of ^{12}C as well as that of other heavy elements. So, precise quantitative measurement of all direct processes (deviation from sequential) in Hoyle state decay is crucially important from nuclear structure as well as astrophysics points of view.

In recent years, quite a few experiments have been performed to investigate and quantify the roles of various decay modes, i.e., sequential decay (SD) and 3α direct decay (DD). In addition, attempts have also been made to identify and differentiate among various types of direct decays, such as decay into equal energies (DDE), decay into a linear chain (DDL), and direct decay in phase space (DD \square), and to quantify their contributions, which are supposed to throw new light on the exotic structure of the Hoyle state.



A complete kinematical measurement of inelastic scattering of α beam of 60 MeV from Variable Energy Cyclotron (VEC) machine on ^{12}C target at 60 MeV to study the various decay channels of Hoyle state with relatively higher in statistic compare to the previous measurement.

Superconducting Magnetic Energy Storage (SMES) system based Dynamic Voltage Restorer:

The Power Quality is one of the most important issues in power distribution system. The problems generally appear in the form of three broad categories that are voltage sags, transients and harmonics. Many critical machines or industrial processes, especially controlled by computers are sensitive to any voltage sag or short interruptions in supplying. These disturbances in supply can increase the down time of the machine and hence the cost of production. Accelerator laboratories also suffer from sudden voltage dip that leads to sub-system trips resulting in shutdown of the entire machine. VECC has undertaken the



development of Superconducting Magnetic Energy Storage (SMES) system based Dynamic Voltage Restorer (DVR) to address this issue that may find application in particle accelerator facilities, R&D laboratories and industries in the country.

DVR (Fig. 1) is one of the most effective and efficient compensating type power electronic controller used in the distribution network to get rid of or to mitigate the most severe power quality problem caused by voltage sags, especially for sensitive loads. Its major components, designed and developed at VECC includes

SMES Coil: The cryostable superconducting magnet was constructed using NbTi based superconductor and High Temperature Superconductor (BSCCO-2223) based electrical current leads to carry DC current of 800Amax, thus storing 0.6MJ of energy. The coil assembly was being housed inside a Standard Magnet Dewar (SMD) with all related instrumentations and coil protection system comprising of a quench detection circuit and dump resistor (20 m-ohm, 5kW) placed externally.

2-Quadrant DC-DC Chopper: A high current IGBT based DC- DC chopper was designed and developed for charging the superconducting coil to its constant current (400A max.) for energy storage and to discharge the stored energy to a constant DC-link capacitor voltage of ~80V as required by the VSI. A novel topology of “Hysteresis Band Controller” was adopted for proper functioning of the chopper in two-quadrant in order to match the power flow demand of the DVR system.

Voltage Source Inverter (VSI) with DSP based control: A 10kVA 3- ϕ VSI was designed and developed that compensates for the voltage sag in the utility mains so as to keep the load voltage constant, deriving power from the chopper controlled constant DC bus. A 12-bit multi-channel 12.5 MSPS ADC and 3- ϕ P.T based instrumentation samples the input mains and feeds to a DSP based controller that ultimately generates the switching signals to the IGBT Bridge of the VSI, employing pre-sag compensation technique.

Harish-Chandra Research Institute (www.hri.res.in)

Several faculty members at HRI received national and international recognition for their research. Among them Prof. Rajesh Gopakumar was awarded the TWAS Physics Prize in October 2013, and the G. D. Birla Prize for scientific research for 2013.

HRI physicists continue to play a key role in the analysis of LHC data. They have also taken a leading role in the collaboration between Indian institutions and the Fermilab, USA, and participate in the Long Baseline Neutrino Experiments (LBNE). The HRI string theory group has



worked on the application of string theory to practical issues in cosmology, hydrodynamics and condensed matter physics. Additionally, there have been formal developments on gauge theories, higher derivative corrections to string theory, and duality between two dimensional quantum field theories and theories of gravity. In condensed matter, there is continuing work on nanomaterials as well as exploration of topological insulators, superconductors and Mott insulators. The quantum information/computation group has explored aspects of non equilibrium many body systems as relevant for quantum information.

The mathematics group at HRI has contributed significantly in research and also through one of the more vibrant outreach programmes in the country. A number of schools, workshops etc. have rejuvenated mathematics learning at college and university levels. This has led to the generation of a pool of manpower trained in current topics in mathematics who are not only trained to start a research career but are also able to contribute significantly in different areas of science and engineering. Recent research work involves developments in the areas of analysis and geometry, Lie groups, and number theory.

Saha Institute of Nuclear Physics (www.saha.ac.in)

Fusion with Anticodon Binding Domain of GluRS is Not Sufficient to Alter the Substrate Specificity of a Chimeric Glu-Q-RS: Glutamyl-queuosine-tRNA(Asp) synthetase (Glu-Q-RS) is a paralog of glutamyl-tRNA synthetase (GluRS) and is found in more than forty species of proteobacteria, cyanobacteria, and actinobacteria. Glu-Q-RS shows striking structural similarity with N-terminal catalytic domain of GluRS (NGluRS) but it lacks the C-terminal anticodon binding domain (CGluRS). In spite of structural similarities, Glu-Q-RS and NGluRS differ in their functional properties. Glu-Q-RS glutamylates the Q34 nucleotide of the anticodon of tRNA(Asp) whereas NGluRS constitutes the catalytic domain of GluRS catalyzing the transfer of Glu on the acceptor end of tRNA(Glu). Since NGluRS is able to catalyze aminoacylation of only tRNA(Glu) the glutamylation capacity of tRNA(Asp) by Glu-Q-RS is surprising. To understand the substrate specificity of Glu-Q-RS we undertook a systemic approach by investigating the biophysical and biochemical properties of the NGluRS (1-301), CGluRS (314-471) and Glu-Q-RS-CGluRS, (1-298 of Glu-Q-RS fused to 314-471 from GluRS). Circular dichroism, fluorescence spectroscopy and differential scanning calorimetry analyses revealed absence of N-terminal domain (1-298 of Glu-Q-RS) and C-terminal domain (314-471 from GluRS) communication in chimera, in contrast to the native full length GluRS. The chimeric Glu-Q-RS is still able to aminoacylate tRNA(Asp) but has also the capacity to bind tRNA(Glu). However the chimeric protein is unable to aminoacylate tRNA(Glu) probably as a consequence of the lack of domain-domain communication.



Doping a Correlated Band Insulator: A New Route to Half-Metallic Behavior: Applying a simple model the surprising result that turning on an on-site Coulomb interaction U in a doped band insulator leads to the formation of a half-metallic state is demonstrated. In the undoped system, we show that increasing U leads to a first order transition at a finite value U -AF between a paramagnetic band insulator and an antiferromagnetic Mott insulator. Upon doping, the system exhibits half-metallic ferrimagnetism over a wide range of doping and interaction strengths on either side of U -AF. Our results, based on dynamical mean field theory, suggest a new route to half metallicity, and will hopefully motivate searches for new materials for spintronics.

Positron annihilation studies of vacancy-type defects and room temperature ferromagnetism in chemically synthesized Li-doped ZnO nanocrystals: The effects of Li incorporation on the lattice defects and Room temperature $d(0)$ ferromagnetic behaviour in ZnO nanocrystals by correlating X-ray photoelectron, photoluminescence and positron annihilation spectroscopic is studied. It is found that at low doping level (≤ 7 at.%), Li^{1+} is an effective substituent of Zn site, but it prefers to occupy the interstitial positions when Li-doping exceeds 7 at.% resulting in lattice expansion and increase of particle sizes. The pristine ZnO nanocrystals exhibit ferromagnetic behaviour which is further enhanced significantly after few percentage of Li-doping in ZnO. The magnitude of both saturation magnetizations (M - S) as well as the Curie temperature (T - C) are found to increase considerably up to Li concentration of 10 at.% and then started to decrease on further Li-doping. The gradual enhancement of Zn vacancy (V -Zn) defects in ZnO nanocrystals due to Li substitution as confirmed from photoluminescence and positron annihilation spectroscopy measurements might be responsible to induce paramagnetic moments within ZnO host. The ferromagnetic exchange interaction between the localised moments of V -Zn defects can be mediated through the holes arising due to Li-substitutional (Li -Zn) acceptor defects within ZnO. Hence, Li doping in ZnO favours in stabilizing considerable V -Zn defects and thus helps to sustain long-range high- T_C ferromagnetism in ZnO which can be a promising material in future spintronics.

Velocity shear effect on the longitudinal wave in a strongly coupled dusty plasma: The characteristics of longitudinal dust acoustic wave (DAW) in presence of velocity shear have been investigated in a strongly coupled dusty plasma using the generalized hydrodynamic (GH) model. In the hydrodynamic regime ($\omega \ll \nu$) (ν is a parts per thousand ν), i.e. when characteristic time τ (ν) is slower than inverse of wave frequency, the viscosity in the GH model plays the usual role of wave damping, whereas in the kinetic regime ($\omega \gg \nu$) (ν is a parts per thousand $\nu \gg 1$), i.e. when characteristic time τ (ν) is larger than inverse of wave frequency, viscosity shows energy storing property in the wave. In the kinetic regime, we have studied the longitudinal mode (where ω is the frequency, k is the wave number, c (d) is the dust acoustic velocity and c (l) is the longitudinal velocity that arises due to viscosity) in



presence of velocity shear. It is shown that velocity shear can destabilize this mode. Both nonmodal and modal techniques are employed to demonstrate the growth rate of the instability.

Inner-most stable circular orbits in extremal and non-extremal Kerr-Taub-NUT spacetimes:

We study causal geodesics in the equatorial plane of the extremal Kerr-Taub-NUT spacetime, focusing on the inner-most stable circular orbit (ISCO), and we compare its behavior with extant results for the ISCO in the extremal Kerr spacetime. Calculations of the radii of the direct ISCO, its Kepler frequency, and the rotational velocity show that the ISCO coincides with the horizon in the exactly extremal situation. We also study geodesics in the strong non-extremal limit, i.e., in the limit of a vanishing Kerr parameter (i.e., for Taub-NUT and massless Taub-NUT spacetimes as special cases of this spacetime). It is shown that the radius of the direct ISCO increases with NUT charge in Taub-NUT spacetime. As a corollary, it is shown that there is no stable circular orbit in massless NUT spacetimes for timelike geodesics.

Institute of Physics (www.iopb.res.in/index.php.php#)

During the year 2013-2014, the Institute of Physics undertook active research in various areas of theoretical and experimental physics. There were seventy publications in refereed journals and proceedings whereas nearly twenty articles were submitted for publication. Six colloquia and sixty one seminars were given by visitors at IOP. Fifty talks were given by the Institute members at various places within the country and abroad.

As in the past, the Institute contributed in a significant way towards quality human resource development in the form of a one year pre-doctoral course followed by the Ph.D. program. Ten post-doctoral fellows joined the Institute in the year 2013-14. Further, this year eight doctoral scholars received their Ph.D. degrees, while eleven scholars joined the pre-doctoral programme. The Institute actively promoted interactions with colleges, universities, academic institutions, and other national laboratories by means of visitor programmes, workshops, symposia, and other academic events.

The Institute organized the 3rd International Conference on Physics at Surfaces and Interfaces (PSI-2014) during February 24 – 28, 2014, International School and Conference on Quantum Information (IPQI-2014) during February 17 – 28, 2014, Discussion Meeting on Radiative Corrections (DMRC) during March 3 – 5, 2014, and co-organized Workshop on High Energy Physics (WHEP-2013) during 12 – 21 December, 2013 as well as National String Meeting during December 2013.



The Institute was also actively involved in popularizing science. The National Science Day was celebrated and students from different schools, across Odisha and Jawahar Navodaya Vidyalayas, visited Institute at different times. In addition, Summer Students' Visiting programme (SSVP – 2013) was organized during May 6 – June 15, 2012 and ten students participated in the same.

Research activities undertaken in the Institute during the year 2013–14 are summarized below.

Condensed Matter Theory: Research activities in condensed matter theory ranged from mesoscopic systems, non-equilibrium statistical mechanics to biophysics. Research was carried out on fluctuation theorems, engines at nano scale, thermodynamics of information, various phase transitions and physical properties especially elastic behaviour of DNA, both in equilibrium and nonequilibrium, and fluctuation induced phases in polymers.

High Energy Physics (HEP) Theory: Research in HEP theory covered areas of HEP phenomenology, string theory, gravity, astro-particle physics, and physics of quark-gluon plasma. Some of the topics of recent interest are gauge / gravity duality, anisotropic power law inflation, black holes and fuzzballs, in particular integrability based techniques for the construction of novel black holes and fuzzballs in supergravity theories, different aspects of relativistic heavy ion collisions, and dual superconductor model of Hadronization. Connection between phase transition in cosmology and Condensed matter system such as liquid crystals, QCD phase transitions in neutron star cores, were investigated. In high energy phenomenology, cross section processes of one loop which are important for analysis of LHC data have been studied. Research was carried out on neutrino oscillation phenomenology with neutrino beams, solar and atmospheric neutrinos, reactor neutrinos, phenomenology with sterile neutrinos, direct and indirect searches of dark matter. There was also active participation in the India-based Neutrino Observatory project

Nuclear Physics Theory: In nuclear Physics, research has focused on nuclear structure and nuclear reaction. The mechanism for the formation of superheavy elements in astrophysical objects, nucleus-nucleus reaction, study of cluster decay properties have been pursued. Recently discovered superheavy nuclei and a new mode of fission decay for neutron-rich heavy nuclei has been studied. Measurement of charged particle multiplicity and transverse energy at mid-rapidity and elliptic flow in Pb-Pb and P-Pb Collisions at 2.76 and 5 TeV with ALICE detector at CERN, LHC are reported. Dynamical observable study in heavy-ion collisions is carried out for

Delta* analysis for p-p at 7 TeV and for p-Pb at 5.02 TeV, Ks* and Lambda analysis at RHIC energies. Work was also carried out on nuclear equation of state of confined and deconfined



matter, nuclear astrophysics, such as compact stars in presence of strong magnetic field, flavor unification, dark matter, and proton decay.

In addition, studies on quantum information were also carried out.

Experimental Physics: In experimental physics, major activities included studies on accelerator based materials science, surface and interface physics, and nano systems. Investigations in these areas were carried out by using the state-of-the-art facilities developed at Institute of Physics over the years. Some of the topics of current interest are ion beam-induced surface nanostructuring, pattern formation, epitaxial crystallization, and electronic structure studies of multiferroics, manganites etc.

Institute for Plasma Research (www.ipr.res.in)

A steady state tokamak **SST-1**- the first of it's kind in India, has been just set up, to study issues related to energy, particle and impurity confinement during steady state operation. Plasma disruptions and vertical displacement episodes will be studied. Non-inductive current drive would sustain the plasma current, and different aspects of the current drive would be studied. The prototype fabrication of the components of the various subsystems of the tokamak has been completed, tested and integrated. SST1 magnets have been activated and the 1st plasma in SST1 was obtained in June 2013. Subsequent plasma experiments in SST1 relates to extending the plasma duration with enhanced current and magnetic field. With the plasma formation in SST1, India is put in the list of six nations globally, that have an operational superconducting tokamak.

Institute of Mathematical Sciences (www.imsc.res.in)

Work done in mathematics is in the areas of algebra, algebraic geometry, algebraic, analytic and transcendental number theory and modular forms, Lie groups, topology, representation theory and operator algebras. This is evidenced by the many publications in these areas and two books. Among the several areas of physics in which research is carried out here are astro-particle physics, biological physics, condensed matter physics, CP-violation, neutrinos, B-physics and new models, foundations of quantum mechanics, mathematical physics, non-linear dynamics, solitons and chaos theory, quantum and topological quantum field theories and conformal field theories, quantum computation and statistical mechanics as evidenced by the publications in all these areas and a book. Theoretical computer science: The main areas of computer science represented here are algorithms and data structures, automata, logic and concurrency, computational complexity and graph theory and combinatorics. Contributions to each of these areas have been made in the form of both journal publications and prestigious conference proceedings.



Tata Memorial Centre (www.tatamemorialcentre.com/education/profedu.htm)

Clinical cancer research has been a major activity at TMC. This has led to two major practice changing research outputs. The first is breast cancer research that has capability of saving thousands of lives by single injection of progesterone given few days prior to surgery. The second is Visual Inspection after application of Acetic Acid (VIA), a public health intervention, which has shown capability of saving over 22000 lives in India and has been adopted by 11 states across our country and has been lauded for its ease of implementation throughout the world. Futility of expensive and exhaustive follow up investigations was investigated for bone and soft tissue tumours and has been a landmark paper in orthopaedic oncology.

The Centre honoured Dr. Prakash Amte and Dr. Mandakini Amte of the Lok Biradari Prakalp, Hemalkasa, with the Science & Society Oration Award – 2013 on 8th April 2013. On 15th August 2013, patient registration services were started at the Hospital in ACTREC, which has enabled treatment of cancer patients from Navi Mumbai and Raigad districts at the centre. In September 2013, a Digital Subtraction Angiography (DSA - Cathlab) facility donated by a philanthropic trust was commissioned in ACTREC. It provides advanced image guided interventional radiology for diagnostic/therapeutic procedures. A new addition to the Cancer Research Institute at ACTREC is the 'Fly lab' which has been set up in August 2013. It aims to utilize Drosophila as a model system to study the signaling pathways regulating glial cell growth and development. During 2013, a state-of-the art core imaging facility has also been established in CRI – ACTREC. It houses 3i Spinning Disk, STED 3X super resolution and multiphoton microscopes that will facilitate cell imaging in multicolor at superfast speed. ACTREC played host to several national and international conferences during 2013 – an important one being the International Symposium on 'Conceptual advances in cellular homeostasis regulated by proteases and chaperones'. Graduate students of the Centre organized the 9th National Research Scholars Meet – 2013 in which a large number of researchers from institutes and universities across the country participated.



Events at Constituent Institutions

Bhabha Atomic Research Centre (www.barc.gov.in)



Graduation function of OCES-2012 OCDF-2012 of BARC Training School, Mumbai. Predisident of India graced the occasion as the chief guest.



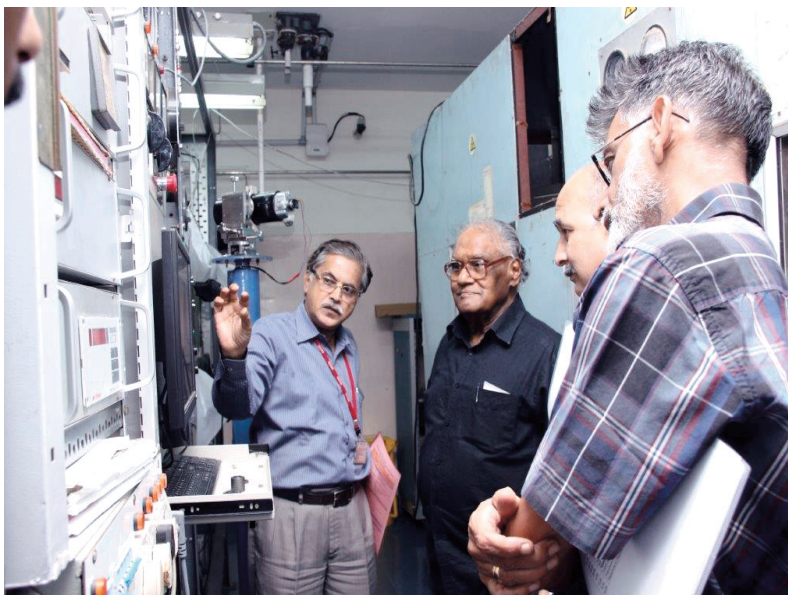
Students & teachers from local colleges attending popular science lectures & exhibitions at BARC during CHEMFEST-2014



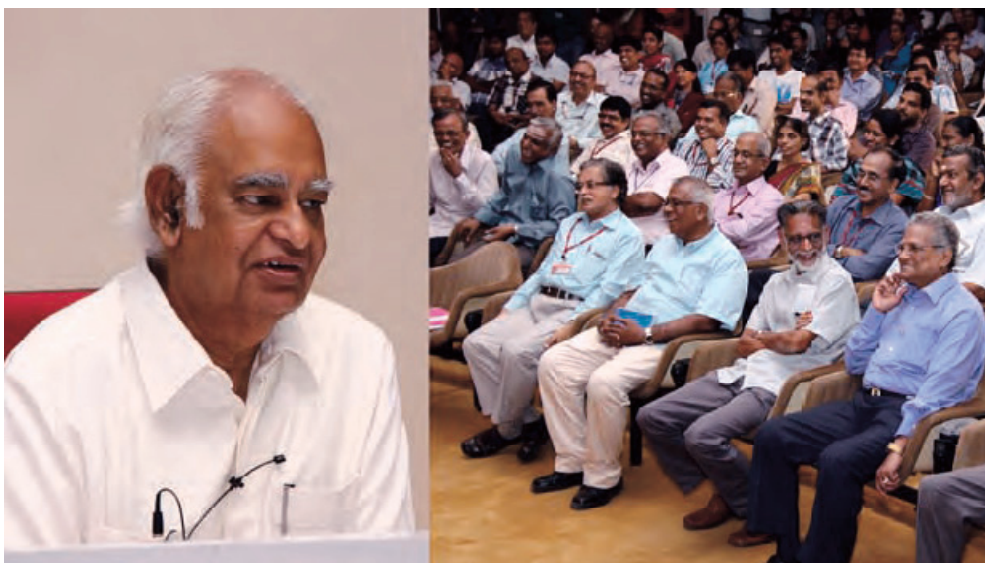
Indocrypt is an International Conference on Cryptology held each year since 2000 in India. Indocrypt 2013 was hosted by Homi Bhabha National Institute during 7-10 December 2013 in Mumbai. The conference was inaugurated by Dr. P. Chidambaram, Principal Scientific Advisor, Government of India. Dr. B. K. Dutta, Dean HBNi and Shri Y. S. Mayya, BARC were conveners.



Indira Gandhi Centre for Atomic Research (www.igcar.gov.in)



Prof. C.N.R. Rao's visit to Chemistry Group, IGCAR



Dr. G. Venkataraman, Director (Retd.) ANURAG, DRDO delivering the IGC Colloquium



Raja Ramanna Centre for Advanced Technology (www.rrcat.gov.in)



Graduation day function of the 13th batch of BARC Training School RRCAT on July 26, 2013; graduating TSOs with the Chief Guest Dr. R. K. Sinha, Chairman, AEC and other dignitaries

Variable Energy Cyclotron Centre (www.vecc.gov.in)



6th Asian Nuclear Physics Association Symposium organized by VECC



VECC organized a summer school on “Nuclear Fission and Related Phenomena” during May 13-23, 2014 to celebrate the 75 years of the discovery of nuclear fission

Harish-Chandra Research Institute (www.hri.res.in)



Prof. Joseph Osterlé, University of Paris, France delivering lecture at HRI Talent Search Prize distribution Function.



Group Photograph of the participants of Instructional School on Schur Multiplier and Related Topics organized at HRI (March 1-8, 2014)



Group Photograph of the participants of the Meeting on Quantum Information Processing and Applications organized at HRI (December 2 - 8, 2013)



Group Photograph of the participants of Instructional School on Schur Multiplier and Related Topics organized at HRI (March 1-8, 2014)



Institute of Physics (www.iopb.res.in/index.php.php#)



Discussion Meeting on Radiative Corrections, March 5-10, 2014, IoP



*3rd International Conference on Physics at Surfaces and Interfaces,
Organized by IoP during Feb.24-28, 201 at Puri*



Institute of Mathematical Sciences (www.imsc.res.in)



Advanced school on Parameterized Complexity and Kernelization at IMSc



Enriching collegiate mathematics workshop at IMSc



Tata Memorial Centre (www.tatamemorialcentre.com/education/profedu.htm)



1st ACTREC Symposium on 'Clinical Pharmacology in Cancer Therapeutics'. Organizer : Dr. Vikram Gote, ACTREC : 19th & 20th April, 2013



International Symposium on 'Conceptual advances in cellular homeostasis regulated by proteases and chaperones' Organizer : Dr. Prasanna Venkatraman, ACTREC : 3rd to 6th December, 2013



9th National Research Scholars meet in Life Sciences 2013 Organisers : Research Scholars, ACTREC : 20th & 21st December, 2013



DPT Workshop on 'Application in Bioinformatics' Organizer : Dr. Ashok Varma, ACTREC : 24th January, 2014

**Conferences Organized by CIs**

Sr. No.	Name of Conference	Organized by (CI)	Venue	Period	
				From	To
1.	Course on Vacuum Science, Technology and Applications	BARC	Gitam University, Vishakhapatnam	24/09/2013	27/09/2013
2.	DAE-BRNS Symposium on Current Trends in Theoretical Chemistry (CTTC 2013)	BARC	Mumbai	26/09/2013	28/09/2013
3.	Workshop cum Training on Nuclear Material Control and Accounting Practices and future Prospective (NUMAC-PP 2013)	BARC	Mumbai	03/10/2013	04/10/2013
4.	Advances in Reactor Physics; Simulation Techniques and Analysis Methodologies	BARC	Training School Hostel, Anushaktinagar, Mumbai	23/10/2013	25/10/2013
5.	Theme Meeting on Ultrafast Sciences (UFS-2013)	BARC	IIT Kharagpur, Kharagpur, West Bengal	25/10/2013	26/10/2013
6.	DAE-BRNS National Symposium on Nuclear Instrumentation 2013 (NSNI-2013)	BARC	Training School Hostel, Anushaktinagar, Mumbai	19/11/2013	21/11/2013
7.	National Workshop on Materials Chemistry (Catalytic Materials)	BARC	Training School Hostel, Anushaktinagar, Mumbai	22/11/2013	23/11/2013
8.	National Symposium on VHE Gamma Ray Astronomy	BARC	Training School Hostel, Anushaktinagar, Mumbai	25/11/2013	27/11/2013
9.	9 th DAE-BRNS Symposium on Current Advances in Immunobiology and Cancer (LSS-2013)	BARC	Training School Hostel, Anushaktinagar, Mumbai	28/11/2013	30/11/2013
10.	Life Sciences Symposium 2013(Current Advances in Immuno Biology & Cancer)	BARC	BARC, Mumbai	28/11/2013	30/11/2013
11.	International Symposium on Nuclear Physics	BARC	Nabhakiya Urja Bhavan, Mumbai	02/12/2013	06/12/2013



12.	DAE-BRNS Nineteenth National Symposium and Workshop on Thermal Analysis (THERMANS 2013)	BARC	Annamalai University, Annamalai Nagar 608 002, Cuddalore District, Tamil Nadu	09/12/2013	13/12/2013
13.	XXXXV Annual Conference of Society of Nuclear Medicine India (SNMICON-2013)	BARC	Nehru Centre, Worli, Mumbai	12/12/2013	15/12/2013
14.	Advances in Radiation Technology for Societal Benefits	BARC	Nabhakiya Urja Bhavan, Mumbai	16/12/2013	18/12/2013
15.	DAE-SOLID STATE PHYSICS SYMPOSIUM 2013	BARC	Thapar University, Patiala, Punjab	17/12/2013	21/12/2013
16.	19 th Symposium and Workshop on Thermal Analysis (Thermans 2013)	BARC	Mumbai	19/12/2013	21/12/2013
17.	Trombay Symposium on radiation and Photochemistry (TSRP-2013)	BARC	Mumbai	06/01/2014	09/01/2014
18.	12th Biennial Trombay Symposium on Radiation and Photochemistry (TSRP-2014)	BARC	Mumbai,	06/01/2014	09/01/2014
19.	New Horizons in Nuclear Reactor thermal Hydraulics and Safety	BARC	Nabhakiya Urja Bhavan, Mumbai	13/01/2014	15/01/2014
20.	DAE-BRNS Symposium on Nuclear Analytical Chemistry (NAC-V)	BARC	BARC, Mumbai	20/01/2014	24/01/2014
21.	5th Symposium on Nuclear Analytical Chemistry (NAC-V)	BARC	BARC, Training School Hostel, Anushaktinagar	20/01/2014	24/01/2014
22.	SFRR Annual Meeting	BARC	Treasure Island Resort, Karla, Lonavala	27/01/2014	30/01/2014
23.	Recent Trends in Free Radical and Antioxidant Research	BARC	BARC, Training School Hostel, Anushaktinagar	27/01/2014	30/01/2014



24.	11 th International Discussion Meet on Electrochemistry and its applications	BARC	Amritsar, Punjab	20/02/2014	25/02/2014
25.	Molecular Architecture, Dynamics and Assembly in Living Systems (MADALS 2014)	BARC	Radisson Blu Hotel, Amritsar	20/02/2014	25/02/2014
26.	DAE-BRNS Symposium on Emerging Trends in Separation Science and Technology	BARC	Mumbai	25/02/2014	28/02/2014
27.	DAE-BRNS Symposium on Organic Devices : The Future Ahead (ODeFA-2014)	BARC	BARC, Training School Hostel, Anushaktinagar	03/03/2014	06/03/2014
28.	International Conference on Advanced Technologies for Management of Ballast Water & Biofouling (MABB 2014)	BARC	Sagar Sangamam complex, NIOT Campus, Chennai 600100	04/03/2014	07/03/2014
29.	28 th ISMAS Workshop cum Symposium on Mass Spectrometry	BARC	Parwanu, HP	09/03/2014	14/03/2014
30.	Orientation course on Environmental Impact Assessment of Nuclear Fuel Cycle Facilities	IGCAR	SRI Seminar Hall, Anupuram	08/07/2013	12/07/2013
31.	DAE-BRNS 7th National Symposium on Pulsed Laser Deposition of thinfilms and Nanostructure Materials (PLD 2013)	IGCAR	IIT, Kharagpur	14/11/2013	16/11/2013
32.	Nuclear Engineering - Future & prospects	IGCAR	Central Leather Research Institute, Chennai 600 020	07/01/2014	08/01/2014
33.	Facilities for handling Radioactive Materials (FRAME 2014)	IGCAR	HASL Lecture Hall, IGCAR, Kalpakkam	22/01/2014	22/01/2014
34.	First International Conference on Structural Integrity (ICONS-2014)	IGCAR	Indira Gandhi Centre for Atomic Research, Kalpakkam	04/02/2014	07/02/2014



35.	Indus Synchrotron Source Utilization Meeting: Photoelectron spectroscopy	RRCAT	RRCAT, Indore	29/08/2013	30/08/2013
36.	Indus Synchrotron Source Utilization Meeting : X-ray Lithography and Microfabrication	RRCAT	RRCAT, Indore	05/12/2013	06/12/2013
37.	School on "Basics of Magnetism and investigations of magnetic properties of materials using Synchrotron Radiation"	RRCAT	RRCAT, Indore	24/03/2014	28/03/2014
38.	International Seminar on Application of Communication and Information Technology in Library (SACITiL)	VECC	Kolkata	28/01/2013	30/01/2013
39.	DAE-BRNS Indian Particle Accelerator Conference 2013	VECC	Kolkata	19/11/2013	22/11/2013
40.	Workshop on Prevention & Response to Nuclear/Radiological Emergencies	VECC	Kolkata	06/02/2014	07/02/2014
41.	6th Asian Nuclear Physics Association Symposium	VECC	Kolkata	19/02/2014	21/02/2014
42.	International Conference on Electron Microscopy	SINP	Hyatt Regency, Kolkata	03/07/2013	05/07/2013
43.	National workshop on Exploring radiation in many splendors (RAD2013)	SINP	Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata 700064	23/11/2013	24/11/2013
44.	The Third International Conference, "Application of RadiotraCers and Energetic Beams in Sciences (ARCEBS-14)	SINP	Kolkata	12/01/2014	18/01/2014



45.	Molecular Architecture, Dynamics and Assembly in Living Systems (MADALS 2014)	SINP	Saha Institute of Nuclear Physics	07/02/2014	10/02/2014
46.	National Symposium on High Power RF & Microwave (HPRFM-2013)	IPR	IPR	04/09/2013	06/09/2013
47.	Topical Conference on Atomic Processes in Plasmas (ISAMP-TC-2013)	ISAMP-IPR	IPR	18/11/2013	20/11/2013
48.	School on Advanced Characterization methods for Nanophase Materials (ACNM-2013)	IPR	IPR	22/11/2013	24/11/2013
49.	School on Nanoscale Excitations in Emergent Materials (NEEM 2013)	IPR	IPR	25/11/2013	26/11/2013
50.	STAR Regional meeting and Discussion on Phases of QCD	IOP and NISER	IOP and NISER	08/07/2013	10/07/2013
51.	International Program on Quantum Information	IOP	IOP	17/02/2014	28/02/2014
52.	3rd International Conference on Physics at Surfaces and Interfaces. PSI2014	IOP	Puri	24/02/2014	28/02/2014
53.	Discussion meeting on radiative corrections	IOP	IOP	05/03/2014	10/03/2014
54.	Workshop & Discussion Meeting (I) Automorphic Forms & Number Theory	HRI	HRI, Allahabad	30/08/2013	03/09/2013
55.	Instructional School on Real Variable Methods in Harmonic Analysis	HRI	HRI, Allahabad	13/09/2013	30/09/2013
56.	Advanced Instructional School on "Real Variable Methods in Harmonic Analysis"	HRI	HRI, Allahabad	23/09/2013	30/09/2013



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57.	Advanced Instructional School for Lecturers- "Topology and Geometry"	HRI	HRI, Allahabad	16/12/2013	28/12/2013
58.	Discussion Meeting on 'Algebraic Curves' (II)	HRI	HRI, Allahabad	19/02/2014	05/03/2014
59.	Instructional School on Schur Multiplier (GTLT)	HRI	HRI, Allahabad	01/03/2014	08/03/2014



Colloquia Organized by CIs

Sr. No.	Speaker	CI	Date	Title
1.	Nandita Maiti	BARC	17/4/2013	Surface-enhanced Raman scattering studies of dimercaptiothiadiazole adsorbed on silver and gold nanoparticles
2.	Sumit Kumar	BARC	12/04/2013	Actinide Speciation
3.	P. S. Ramanjeyulu	BARC	24/04/2013	Development of methodology for the determination of boron in ThO ₂ employing spectrophotometry
4.	Sisir K. Sarkar	BARC	25/04/2013	Coherent Control : Replacing Serendipity with Intention
5.	Rajib Ghosh	BARC	15/05/2013	Ultrafast Structural Relaxation Dynamics of Donor-Acceptor Ketone Derivatives
6.	Neetika Rawat	BARC	24/05/2013	Thermodynamics of actinide complexation reactions
7.	Manjulata Sahoo	BARC	07/06/2013	Physico-chemico properties of Cr ₂ TeO ₆ (s), Fe ₂ TeO ₆ (s) and Ni ₃ TeO ₆ (s)
8.	Ashwani Kumar	BARC	21/06/2013	Non-destructive assay of nuclear materials
9.	Sudhir Kappoor	BARC	02/07/2013	Zeolite Materials: Preparation of Metal Nanoparticles and Selective Catalysis
10.	R.N. Singh	BARC	11/07/2013	Hydrogen in Zr-alloys and its consequences in life management of in-core components of PHWR
11.	S. Jeyakumar	BARC	13/07/2013	Ion Chromatographic analysis of trace elements in nuclear materials
12.	J. Manjanna	BARC	26/07/2013	Diffusion of traces in altered clay minerals relevant to deep geological disposal of HLW.
13.	V. G. Mishra	BARC	16/08/2013	Determination of stability constants of tetracycline complexation with Zr and Hf
14.	Biswajit Manna	BARC	04/09/2013	Study of Exciton Dynamics in Polyacene Nanoaggregates
15.	Ankita Rao	BARC	04/09/2013	Supercritical fluid extraction of actinides
16.	Atanu Barik	BARC	13/10/2013	One-electron redox reaction of organo-selenium compounds: A pulse radiolysis study
17.	Prabhat K. Singh	BARC	06/11/2013	Exploring Nano-confined water using a symmetric Ion: A 2D IR Investigation
18.	Prakash D. Naik	BARC	25/11/2013	Laser Spectroscopy In Analytical Chemistry
19.	B.S. Tomar	BARC	02/12/2013	Radiation Detection and Measurements



20.	M. C. Rath	BARC	11/12/2013	Radiation and Photochemistry in Nuclear Industry: A New Horizon
21.	S. Venugopal Rao	BARC	18/12/2013	Ultrafast ablation, LIBS and pump-probe techniques for studying high energy materials
22.	P.N. Raju	BARC	03/02/2014	Role of Statistics in Nuclear Material Accounting & Control
23.	Arijit Kumar De	BARC	19/03/2013	Probing ultrafast coherent dynamics by incoherent fluorescence detection: Towards a spatiotemporal approach
24.	John Philip	BARC	17/05/2013	SMART NANO MATERIALS- SCIENCE AND APPLICATIONS
25.	N.Sivaraman	BARC	01/07/2013	SEPARATION TECHNIQUES
26.	Prof. Deshdeep Sahdev , IIT, Kanpur	RRCAT	18/09/2013	Quantum Mechanics and Solid State Physics with an Indigenous STM and Physical Quantities Measurement System
27.	Dr. Venuka D. Goyal, IIT Bombay	RRCAT	09/10/2013	Protein Engineering: Tailoring Enzymes to Suit our Requirements
28.	Dr. Praveen Chaddah, RRCAT	RRCAT	27/11/2013	Ethics in Research and Publications: looking at Plagiarism
29.	Dr. S.P. Mhaskar, Diamond Light Source, UK	RRCAT	29/11/2013	Magnet and insertion devices related activities at Diamond
30.	Prof. Donald Bilderback, Cornell High Energy Synchrotron Source	RRCAT	04/12/2013	Overview of the Cornell High Energy Synchrotron Source (CHESS), upgrade possibilities to Energy Recovery Linac, x-ray experiments, and a perspective on capillary x-ray optics
31.	Prof. A. Yamaguchi, Hyogo University, Japan	RRCAT	06/12/2013	Electrical measurements and real space magnetization dynamics induced by microwave nano magnets
32.	Prof. Edward I. Moses, University of California, Berkeley, and Lawrence Livermore National Laboratory, Livermore, USA	RRCAT	13/12/2013	The National Ignition Facility: Pathway to Energy Security and Physics of the Cosmos
33.	Prof. Shuji Miyamoto, University of Hyogo, Japan	RRCAT	15/12/2013	Gamma-ray Generation and Application by Laser Compton Scatte
34.	Prof. Elias Towe, Carnegie Mellon University, USA	RRCAT	17/12/2013	Mode-locked High Peak Power Photonic Crystal Laser Systems
35.	Dr. Oliver Puncken, The University of Texas at Brownsville, USA,	RRCAT	31/12/2013	Pre-Stabilized Laser System for the Advanced-LIGO Detector



36.	Dr. D. R. M. Samudraiah, ISRO, Ahmedabad	RRCAT	01/08/2014	Remote Sensor Technologies- Challenges in Electro-optical Sensors Development
37.	Mr. Rakesh Kaul, RRCAT, Indore	RRCAT	26/02/2014	A Study on Vacuum Brazing of Niobium-Stainless Steel Transition Joint for Application in Superconducting Cavities
38.	Prof. Sunanda Banerjee, SINP, Kolkata	IOP	27/05/2013	New Particle at the Large Hadron Collider
39.	Professor K. Sridhar, Tata Institute of Fundamental Research, Mumbai	IOP	12/08/2013	NRQCD -- How effective a theory of charmonium is it?
40.	Ar. Shakti Nanda, BBSR	IOP	02/09/2013	Journey of a photographer through the green corridors of motherland
41.	Prof. Hans Hofsäss, University Göttingen, Germany	IOP	18/10/2013	Dot and ripple patterns - self organized-ion induced impurity triggered
42.	Dr. Vipin K. Yadav , Planetary Science Branch (PSB) , Space Physics Laboratory (SPL , Vikram Sarabhai Space Centre (VSSC), Thiruvananthapuram	IOP	02/12/2013	Mangalyaan - Indian Mars Orbiter Mission
43.	Dr. Ayan Mukhopadhyay, Postdoctoral Researcher, CPHT Ecole Polytechnique and IPHT CEA-Saclay	IOP	10/12/2013	Applications of the holographic correspondence
44.	Professor Carla Farsi, University of Colorado	HRI	30/04/2013	"Group Actions: a Bridge between Geometry, Algebra and Analysis"
45.	Professor Kaushal Verma, IISc Bangalore	HRI	27/04/2013	"Introduction to complex dynamical systems"
46.	Prof Adimurthi, TIFR CAM, Bangalore	HRI	17/04/2013	"Viscosity Solutions for Hamilton Jacobi (HJ) Equations and its application to Conservation laws"
47.	Prof Adimurthi, TIFR CAM, Bangalore	HRI	19/04/2013	"Viscosity Solutions for Hamilton Jacobi (HJ) Equations and its application to Conservation laws"
48.	Prof Adimurthi, TIFR CAM, Bangalore	HRI	22/04/2013	"Viscosity Solutions for Hamilton Jacobi (HJ) Equations and its application to Conservation laws"
49.	Prof Adimurthi, TIFR CAM, Bangalore	HRI	29/04/2013	"Viscosity Solutions for Hamilton Jacobi (HJ) Equations and its application to Conservation laws"



50.	Dr. Sachin Sharma,HRI	HRI	01-05-2013	"The t-analog of the basic string function for twisted affine Lie algebras"
51.	Professor Carla Farsi, University of Colorado	HRI	02-05-2013	Orbifold and Non--Orbifold Algebras of certain Hamiltonian
52.	Prof Adimurthi, TIFR CAM, Bangalore	HRI	02-05-2013	Viscosity Solutions for Hamilton Jacobi (HJ) Equations and its application to Conservation laws
53.	Prof Adimurthi, TIFR CAM, Bangalore	HRI	05-03-2013	Viscosity Solutions for Hamilton Jacobi (HJ) Equations and its application to Conservation laws
54.	Professor S. Eswara Rao, TIFR Mumbai	HRI	28/5/2013	Classification of irreducible, integrable modules for the full toroidal Lie algebras
55.	Professor TD Browning, University of Bristol	HRI	07/10/2013	A new polynomial sieve and equal sums of like polynomials
56.	Dr. Makoto Minamide, Kyoto Sangyo University, Kyoto	HRI	26/09/2013	On the integral $\int_0^x \frac{t^n}{\sin t} dt$
57.	Prof. S. M. Srivastava, ISI, Kolkata	HRI	02/12/2013 to 03/12/2013	A Solution of Hilbert's Seventeenth Problem - Applications of Logic to Algebra and Geometry
58.	Prof. Shrawan Kumar, University of North Carolina	HRI	12/12/2013	"Hermitian eigenvalue problem and its generalization to any semisimple group: A survey"
59.	Prof. Carlo M. Scoppola, University of L'Aquila, Italy	HRI	13/12/2013	"Pro-p groups"
60.	Prof. P. Vanchinathan,VIT University, Chennai	HRI	24/01/2014	"Chinese Remainder Theorem: Some Applications"
61.	Prof. Mahan Mj,Ram Krishna Vivekanand University, Belur	HRI	27/01/2014	"Low dimensional projective groups" (IMS Colloquium)
62.	Prof. P. Vanchinathan,VIT University, Chennai	HRI	28/01/2014	"Ramanujan and his Spirituality According to Kanigel"
63.	Prof. P. Vanchinathan,VIT University, Chennai	HRI	29/01/2014	"Chinese Remainder Theorem: Some Applications"
64.	Prof. Silvio Dolfi, Italy	HRI	14/02/2014	" Character degrees and conjugacy class sizes of finite groups"
65.	Prof. Ramesh Sreekantan	HRI	04/03/2014	Algebraic Cycles and the Fundamental Group.
66.	Richard Garavuso	HRI	09/04/2013	Deformed mathai-quillen forms in A-twisted (0,2) landau-ginzburg models
67.	Vikram Vyas	HRI	16/04/2013	Heavy-Quark potential: Shadows of five dimensions.



68.	Amit Dutta	HRI	25/04/2013	The Ground State Quantum fidelity; and indicator of quantum criticality
69.	Rakibur Rahman	HRI	03/07/2013	Holographic Constraints On A Vector Boson
70.	Roji Pius	HRI	23/07/2013	Simplest Gauge String Duality
71.	Abhishek Chowdhury	HRI	24/07/2013	Black Hole Bound State Metamorphosis
72.	Swapnamay Mondal	HRI	24/07/2013	Black Hole State counting and supersymmetric quantum mechanics.
73.	Mehendi Masud	HRI	26/07/2013	Study of Different detector configurations in long base line neutrino experiment (LBNE).
74.	Matan Field	HRI	30/07/2013	Low-Energy Effective actions from Holography
75.	Ayan Mukhopadhyay	HRI	05/08/2013	Spacetime emergence via holographic RG flow from incompressible Navier-stokes at the horizon.
76.	Ayan Mukhopadhyay	HRI	06/08/2013	Generalized Landau-Silin theory and Boltzmann-Vlasov equations for semi-holographic non-Fermi liquids.
77.	Arnob Rudra	HRI	07/08/2013	Degeneration of two loop superstring scattering amplitude.
78.	Arunabha Saha	HRI	08/08/2013	Black Holes in 3D higher Spin gravity.
79.	Masahide Manabe	HRI	21/08/2013	Stringy Instanton Counting and Topological Strings.
80.	Yoshinori Honma	HRI	22/08/2013	Kahler Potential for (super) Calabi-Yau Manifold.
81.	Swapnamay Mondal	HRI	05/09/2013	Extinguishing Fire at the event horizon!
82.	Siddarth Dwivedi	HRI	10/09/2013	Forward and inverse algorithms.
83.	Arindam Chatterjee	HRI	27/09/2013	Right-handed sneutrino Dark Matter and the 135 GeV γ ray line
84.	Siddarth Dwivedi	HRI	01/10/2013	Brace Tiling.
85.	Millind Shyani	HRI	05/10/2013	2D Blackholes and the Information Problem.
86.	Deepak Tiwari	HRI	01/11/2013	Indirect searches of Dark Matter signatures at INO
87.	Richard Garavuso	HRI	12/11/2013	Analogues of Mathai-Quillen forms in Sheaf cohomology and applications to topological field theory.
88.	Bobby Ezhuthachan	HRI	26/11/2013	Giant gravitons in $AdS_4 \times S^7/Z_k$
89.	Ambresh Shivaji	HRI	28/11/2013	The effects of top-Higgs anomalous coupling in double Higgs production



90.	Trilochan Bagarti	HRI	03/12/2013	On spin Transport and The Trapping of classical particles
91.	Roji Pius	HRI	05/12/2013	Mass Renormalization in String Theory
92.	Adeline Crépieux	HRI	16/12/2013	Current fluctuations and thermoelectricity in interacting/coupled nano-systems.
93.	P. S. Burada	HRI	17/12/2013	Passive and active transport.
94.	Mireille Lavagna	HRI	17/12/2013	Interacting quantum dots under nonequilibrium condition.
95.	Brajesh Gupt	HRI	14/01/2014	Non-singular AdS-dS transitions in a landscape scenario.
96.	Kaustubh Deshpanday	HRI	14/01/2014	Holographic Schwinger effect and critical electric field strength.
97.	Sovan Chakraborty	HRI	16/01/2014	Probing Lorentz invariance violation with the iceCube PeV neutrinos.
98.	Arijit Saha	HRI	20/01/2014	Transport Signatures of fractional fermions in nanowires.
99.	Deepak Dhar	HRI	21/01/2014	Understanding 1/f noise.
100	Vatsal Dwivedi	HRI	22/01/2014	A kinetic Theory approach to Gauge anomalies.
101	Arjun Menon	HRI	22/01/2014	Searching for neutral Higgs bosons in non-standard channels.
102	Katri Huitu	HRI	30/01/2014	Spontaneous R-parity and/or CP violation in NMSSM with right handed neutrinos.
103	Mariana Frank	HRI	03/02/2014	Charginos and Neutralinos beyond MSSM.
104	Durga Prasad Roy	HRI	10/02/2014	Why LHC?
105	Abhishek Sadhukhan	HRI	11/02/2014	Semiclassical folded spinning string in AdS ₃ .
106	Masazumi Honda	HRI	12/02/2014	Higgs branch localization of 3-D N=2 theories.
107	Durga Prasad Roy	HRI	13/02/2014	Determination of the third mixing angle θ_{13} and its implications.
108	Durga Prasad Roy	HRI	18/02/2014	Phenomenology of non-universal Gaugino mass models.
109	Ashiwin S. Panday	HRI	20/02/2014	KK-Monopoles: A study using topological T-Duality.
110	Tomohisa Takimi	HRI	25/02/2014	Phase structure of the large N Chern-Simons matter theories in the fundamental representation on $S^2 \times S^1$.
111	Arpan Bhattacharya	HRI	26/02/2014	Holographic entanglement entropy.
112	Sven Krippendorf	HRI	03/03/2014	Phenomenology with D-branes at singularities in type IIB string compactifications.



113	Ram Lal Awasthi	HRI	06/03/2014	Beyond Standard Model Physics: A non-SUSY grand unification perspective.
114	Sachin Jain	HRI	21/03/2014	Scattering in Chern simons theories with fundamental matter.
115	K Vijay Kumar, Max Planck Institute for the Physics of Complex Systems, Germany	IMSc	08/04/2013	The cell cortex : A thin film of active matter
116	Nilanjan Sircar TIFR, Mumbai	IMSc	10/04/2013	Extremal Horizons with Reduced Symmetry : Towards Novel Phases of Nature
117	Kamalakshya Mahatab IMSc	IMSc	10/04/2013	Representation-theoretic approach to ADG problem
118	Nilanjan Sircar , TIFR, Mumbai	IMSc	12/04/2013	Extremal Horizons with Reduced Symmetry:Novel Phases of Nature
119	Sachin Sharma , IMSC & HRI	IMSc	15/04/2013	The t-analogue of string functions for the affine Kac-Moody algebras.
120	V Sasidevan, TIFR, Mumbai	IMSc	15/04/2013	Stochastic strategies in Minority game
121	Uday Bhaskar Sharma IMSc	IMSc	17/04/2013	Gabriel's Theorem
122	V Sasidevan, TIFR, Mumbai	IMSc	18/04/2013	A Continuum Percolation Problem
123	Barath Coleppa, University of Arizona	IMSc	19/04/2013	Constraining Models With Strong Top-Quark Dynamics
124	G. Arunkumar, IMSc	IMSc	24/04/2013	Wedderburn's theorem
125	Ekata Saha, IMSc	IMSc	24/04/2013	Hilbert's Nullstellensatz
126	Priyamvad Srivastav, IMSc	IMSc	24/04/2013	The Frobenius Density Theorem
127	P. A. Narayanan, IMSc	IMSc	24/04/2013	Choquet Theorem
128	Kesab Chandra Bakshi, IMSc	IMSc	24/04/2013	Hausdorff measure and its elementary properties
129	Venkata Raghu Tej Pantangji, IMSc	IMSc	24/04/2013	Brauer Induction Theorem



130	Biswajyoti Saha, IMSc	IMSc	24/04/2013	Dimension in finitely generated k-algebra
131	Sohan Lal Sahni, IMSc	IMSc	24/04/2013	Analytic set and Souslin's Theorem
132	Nidhish Unnikrishnan, IMSc	IMSc	24/04/2013	Cardinal and Ordinal Invariants in Topology with reference to Dimension Theory
133	Uday Bhaskar Sharma, IMSc	IMSc	25/04/2013	Gabriel's Theorem
134	Madhusree Basu, IMSc	IMSc	02/05/2013	Continuous Minmax Theorems
135	Krishnan Rajkumar, SNU, Delhi	IMSc	02/05/2013	PhD Thesis Defense
136	Tapas Chatterjee, IMSc	IMSc	04/05/2013	Ph.D Thesis defense talk
137	Samrat Bhowmick, Institute of Physics,	IMSc	19/06/2013	Anisotropic branes
138	Wilberd van der Kallen, Universiteit Utrecht	IMSc	19/06/2013	Cohomological finite generation
139	N.S. Vidhyadhiraja, JNCASR, Bangalore	IMSc	20/06/2013	Non-Fermi liquid behaviour due to Disorder in correlated Fermi liquids
140	Rishi Vyas, University of Cambridge	IMSc	20/06/2013	Introductory homological algebra
141	Krishnendu Sengupta, IACS, Kolkata	IMSc	21/06/2013	Dynamics of the Bose-Hubbard model
142	Wilberd van der Kallen, Universiteit Utrecht	IMSc	21/06/2013	Cohomological finite generation
143	T. S. Subramanian, The Hindu	IMSc	21/06/2013	Discoveries from Khirsara - a new Indus Valley site in Gujarat
144	Rishi Vyas, University of Cambridge	IMSc	21/06/2013	Introductory homological algebra II
145	J. Maharana, Institute of Physics and NISER, Bhubaneswar	IMSc	24/06/2013	T-duality of NSR superstring
146	Wilberd van der Kallen, Universiteit Utrecht	IMSc	24/06/2013	Cohomological finite generation
147	Rishi Vyas, University of Cambridge	IMSc	24/06/2013	Introductory homological algebra III: Spectral sequences
148	Upendra Kulkarni: convener, CMI	IMSc	25/06/2013	Informal discussion
149	Debajyoti Sarkar, City University of New York, NY, USA	IMSc	26/06/2013	Black Hole formation at the Correspondence Point



150.	Wilberd van der Kallen, Universiteit Utrecht	IMSc	27/06/2013	Cohomological finite generation
151.	Jayalal Sarma, IIT Madras	IMSc	28/06/2013	Arithmetic Circuit Lower Bounds via Partial Derivatives Matrix
152.	K N Raghavan: convener, IMSc	IMSc	28/06/2013	Comological finite generation
153.	P. Ravindran, Central University of Tamil Nadu, Thiruvapur	IMSc	03/07/2013	Multifunctional oxides: Design and development from first principle calculations
154.	Wilberd van der Kallen, Universiteit Utrecht	IMSc	03/07/2013	Cohomological finite generation
155.	Informal discussion (convener: K. N. Raghavan) IMSc	IMSc	04/07/2013	Cohomological finite generation
156.	Wilberd van der Kallen, Universiteit Utrecht	IMSc	05/07/2013	Cohomological finite generation
157.	Sankardeep Chakaborty, IMSc	IMSc	08/07/2013	Topics in Correlation Bounds
158.	Wilberd van der Kallen, Universiteit Utrecht	IMSc	08/07/2013	Cohomological finite generation
159.	Travis Scrimshaw, UC Davis	IMSc	08/07/2013	Introduction to Sage
160.	Wilberd van der Kallen, Universiteit Utrecht	IMSc	09/07/2013	Cohomological finite generation
161.	Anil Shukla, IMSc	IMSc	10/07/2013	Resolution Proof Systems
162.	Kajari Mazumdar, TIFR	IMSc	10/07/2013	What next at the LHC?
163.	Ram Murty, Queen's University	IMSc	11/07/2013	The Twin Prime Problem (apres Yitang Zhang)
164.	R. Venkatesh, TIFR, Mumbai	IMSc	11/07/2013	Unique Factorization Of Tensor Products For Kac-Moody Algebras
165.	Uma Sankar, IIT Mumbai	IMSc	12/07/2013	Expectations from Nova
166.	Wilberd van der Kallen. Universiteit Utrecht	IMSc	12/07/2013	Cohomological finite generation
167.	Travis Scrimshaw, UC Davis	IMSc	12/07/2013	Crystals and Rigged Configurations



168.	T Prasad, Ahalia School of Engineering and Technology, Palakkad	IMSc	15/07/2013	Variations of Weyl type theorems and hypercyclic/supercyclic operators
169.	Travis Scrimshaw, UC Davis	IMSc	15/07/2013	Introduction to Sage
170.	Ram Murty, Queen's University	IMSc	16/07/2013	The Goldston-Pintz-Yildirim Theorem
171.	Travis Scrimshaw, UC Davis	IMSc	17/07/2013	Introduction to Sage (part two)
172.	Kamalakhya Mahatab and Kannappan Sampath IMSc, ISI Bangalore	IMSc	17/07/2013	Consequences of Failure of Chinese Remainder Theorem in the Ring of Polynomials over Integers
173.	Ram Murty, Queen's University	IMSc	18/07/2013	Zhang's Theorem
174.	Travis Scrimshaw, UC Davis	IMSc	19/07/2013	Introduction to Sage (part three)
175.	Kamalakhya Mahatab and Kannappan Sampath IMSc, ISI Bangalore	IMSc	19/07/2013	Consequences of Failure of Chinese Remainder Theorem in the Ring of Polynomials over Integers (part two)
176.	Michael Griffin, Emory University	IMSc	22/07/2013	Weierstrass Mock Modular Forms and Elliptic Curves
177.	Travis Scrimshaw, UC Davis	IMSc	22/07/2013	Introduction to Sage (part four)
178.	Anuradha Jagannathan, University of Paris 11, Orsay, France	IMSc	23/07/2013	Introduction to Quasicrystals and Quantum Models
179.	Michael Griffin, Emory University	IMSc	23/07/2013	Mock modular forms
180.	M.S. Raghunathan, IIT Mumbai	IMSc	24/07/2013	Lie Groups
181.	M. S. Raghunathan, IIT Mumbai	IMSc	25/07/2013	Lie Groups
182.	Travis Scrimshaw, UC Davis	IMSc	26/07/2013	Introduction to k-Schur functions
183.	M.S. Raghunathan, IIT Mumbai	IMSc	26/07/2013	Lie Groups



184	M. S. Ramanujan, IMSc	IMSc	29/07/2013	Parameterized Graph Separation Problems: New Techniques and Algorithms
185	Rajarshi Pal, IMSc	IMSc	01/08/2013	Optimal teleportation fidelity of a generic qubit channel
186	AP Balachandran, Syracuse University	IMSc	02/08/2013	Edge States: Topological Insulators, Superconductors
187	Kamalakshya Mahatab, IMSc	IMSc	02/08/2013	Counting Irreducibles in Group Semirings of $Z/2Z$ and $Z/3Z$
188	C. P. Anilkumar, IMSc	IMSc	05/08/2013	Ring of Integers in the biquadratic extension
189	Anupam Kundu, LPTMS, University of Paris-SUD, Orsay	IMSc	07/08/2013	Exact distributions of the number of distinct and common sites visited by N independent random walkers
190	Parimala Raman, Department of Mathematics CS Emory University	IMSc	07/08/2013	Period-index questions for function fields
191	Debtosh Chowdhury, CHEP, IISc, Bangalore	IMSc	07/08/2013	Three roads to SUSY: Impact of direct and indirect searches
192	Karteek Sreenivasaiah, IMSc	IMSc	08/08/2013	Small depth proof systems
193	A.M.M. Pruisken, University of Amsterdam	IMSc	12/08/2013	Friend or Foe ? The quantum criticality observed in the quantum Hall regime
194	V. S. Sunder, IMSc	IMSc	13/08/2013	About the Horn Conjecture
195	Matthew Lunde, UC Riverside	IMSc	13/08/2013	Representation theory of quantum (loop) algebras
196	S. Arulmozhiraja, Bharathiar University, Coimbatore	IMSc	13/08/2013	Is Density Functional Theory Inadequate?
197	E. C. G. Sudarshan and Mark, Selover, Univ. of Texas at Austin	IMSc	14/08/2013	CPT Theorem
198	K. R. Parthasarathy, ISI Delhi	IMSc	14/08/2013	Gaussian states and their symmetry group
199	Matthew Lunde, UC Riverside	IMSc	14/08/2013	Representation theory of quantum (loop) algebras



200	K R Parthasarathy, ISI Delhi	IMSc	16/08/2013	Gaussian states and their symmetry (part 2)
201	Nitin Saurabh	IMSc	22/08/2013	Complexity reading group
202	Jaya Maji, IMSc	IMSc	23/08/2013	Efimov-like states and conformational transitions of DNA
203	Amritanshu Prasad, IMSc	IMSc	23/08/2013	Extensions and orbits of finite abelian groups
204	K R Parthasarathy, Indian Statistical Institute, New Delhi	IMSc	23/08/2013	Gaussian states and their symmetry – III
205	Ayan Mukhopadhyay, Ecole Polytechnique, France	IMSc	23/08/2013	Spacetime emergence from holographic RG flow and the fluid-gravity correspondence
206	Manoj Verma, Post Doctoral Fellow, IMSc	IMSc	29/08/2013	Circle Method
207	M. Praveen, Labri, U. Bordeaux-1	IMSc	30/08/2013	Reasoning about data repetitions with counter systems
208	A.J. Parameswaran, TIFR, Mumbai	IMSc	30/08/2013	On the geometry of regular maps from a quasi-projective surface to a curve
209	Kamal Bardhan, Saha Institute of Nuclear Physics, Kolkata	IMSc	02/09/2013	Universal Scaling in Disordered Systems: tale of nonlinearity exponents
210	Pinaki Banerjee, IMSc	IMSc	03/09/2013	Holographic Brownian motion in 1+1 Dimensions
211	Event Canceled, TIFR, Mumbai	IMSc	04/09/2013	Geometrically frustrated magnetism among spin-chain systems
212	K N Raghavan, IMSc	IMSc	04/09/2013	Semi-invariants of quivers and the saturation conjecture
213	K N Raghavan, IMSc	IMSc	05/09/2013	Semi-invariants of quivers and the saturation conjecture II
214	Dhriti Ranjan Dolai, IMSC Chennai	IMSc	05/09/2013	Random Operator Seminar



215	Manoj Verma, Post Doctoral Fellow, IMSc	IMSc	05/09/2013	Circle Method
216	C. P. Anilkumar, IMSc	IMSc	06/09/2013	Orbit of Pairs in Finite Modules over Discrete Valuation Rings and Permutation Representations
217	B. Ramakrishnan, HRI	IMSc	06/09/2013	Jacobi forms of weight two and restriction map
218	A. J. Parameswaran, TIFR, Mumbai	IMSc	10/09/2013	Picard bundles and Brill-Noether loci in the compactified jacobian of a nodal curve
219	Anirban Mukhopadhyay, IMSc	IMSc	10/09/2013	Twin prime conjecture
220	Debraj Roy, SN Bose National Centre for Basic Sciences	IMSc	11/09/2013	'Trivial Symmetries' in models of gravity
221	K N Raghavan, IMSc	IMSc	11/09/2013	Semi-invariants of quivers and the saturation conjecture
222	R. Chandrashekar, IMSc	IMSc	12/09/2013	Statistical Mechanics based on generalized entropies and its applications
223	Prof S Kotani, Kwansei Gakuin University, Sanda, Japan	IMSc	12/09/2013	On the limit set of KdV flows
224	Arijit Roy, Laufer Center for Physical and Quantitative Biology, Stony Brook University, Stony Brook, NY 11794-5252	IMSc	16/09/2013	A method for calculating conversion free-energies between protein conformations
225	Jainendra Jain, Penn. State Univ., USA	IMSc	16/09/2013	Composite Fermions: The Magical Beauty of Emergence
226	G. Baskaran, IMSc.	IMSc	17/09/2013	Is Silicene a Carbon Copy of Graphene?
227	Anirban Mukhopadhyay, IMSc	IMSc	17/09/2013	Bounded gaps between primes



228	Ramamohan Paturi, University of California, San Diego	IMSc	17/09/2013	Exact Complexity and Satisfiability
229	R. Shankar, IMSc	IMSc	18/09/2013	The Story of Climate Change
230	Anilkumar C. P., IMSc	IMSc	18/09/2013	Orbits of Pairs in Finite Modules over Discrete Valuation Rings and Permutation Representations
231	Manoj Verma, Post Doctoral Fellow, IMSc	IMSc	19/09/2013	Circle Method
232	K R Balakrishnan, Director, Cardiac Sciences, Malar Fortis Hospital, Chennai	IMSc	19/09/2013	Artificial Heart: Current Options
233	N Minami, Keio University	IMSc	19/09/2013	The Stochastic Airy Operators
234	Siddarth Parameswaran, Univ. California, Berkeley	IMSc	20/09/2013	Fractionalization from Crystallography
235	Amritanshu Prasad, IMSc	IMSc	20/09/2013	Similarity classes modulo p^2 and pairs of commuting matrices
236	B P Ajith Kumar, IUAC, New Delhi	IMSc	21/09/2013	Make your computer a science lab
237	Siddarth Parameswaran, Univ. California, Berkeley	IMSc	23/09/2013	A Typology for Topological Liquids
238	Anirban Mukhopadhyay, IMSc	IMSc	24/09/2013	Bounded gaps between primes
239	R. Srinivasan, CMI	IMSc	24/09/2013	E_0 - semigroups on factors
240	Pampa Paul, IMSc	IMSc	25/09/2013	L_0 types common to a Borel-de Siebenthal discrete series and its associated holomorphic discrete series
241	Panchugopal Bikram, IMSc	IMSc	26/09/2013	Extendability of endomorphisms of factors



242	B.V. Rajarama Bhat, ISI, Bangalore	IMSc	26/09/2013	Nilpotent completely positive maps
243	Shivakumar Jolad, IIT Gandhinagar	IMSc	27/09/2013	Modeling spatial patterns of spread of Dengue with Human and Vector Mobility
244	T. Geetha, IMSc	IMSc	27/09/2013	The Structure Constants of the Schur Algebra
245	Indrakshi Raycoudhary, IMSc	IMSc	01/10/2013	Prepotential Formulation of Lattice Gauge Theories
246	R. Srinivasan, CMI	IMSc	01/10/2013	E0 -semigroups on factors-II
247	Sushant Raut, Physical Research Laboratory	IMSc	03/10/2013	Synergies between neutrino oscillation experiments: Economizing future facilities
248	Prabha Mandayam, IMSc	IMSc	03/10/2013	Incompatibility and complementarity in quantum information theory
249	Senthamarai Kannan, CMI	IMSc	04/10/2013	Automorphism group of a smooth Schubert variety
250	T. Geetha, IMSc	IMSc	04/10/2013	Graphic interpretation of structure constants of the Schur algebra
251	Ramesh Sreekantan ISI Bangalore	IMSc	08/10/2013	Higher Chow cycles on Abelian Surfaces
252	Peter Fiebig FAU, Erlangen-Nuernberg	IMSc	09/10/2013	Modular representations of algebraic groups
253	S P Suresh, CMI, Chennai	IMSc	10/10/2013	Primal infor logic: proof theory and efficient decidability
254	Manoj Verma, IMSc	IMSc	10/10/2013	Representation of Integers by a Family of Cubic Forms
255	Peter Fiebig, FAU, Erlangen-Nuernberg	IMSc	15/10/2013	Modular representations of algebraic groups



256.	R. Srinivasan, CMI	IMSc	15/10/2013	E0 - semigroups on factors-III
257.	Gyan Prakash, Harish-Chandra Research Institute	IMSc	15/10/2013	Roth's theorem in primes and its generalisation
258.	Peter Fiebig, FAU, Erlangen-Nuernberg	IMSc	17/10/2013	Modular representations of algebraic groups
259.	Yashonidhi Pandey, IISER, Mohali	IMSc	17/10/2013	Brauer group of moduli of torsors under parahoric group scheme G over a curve
260.	Bobby Ezhuthachan, Vivekananda University, Belur	IMSc	18/10/2013	Giant gravitons in AdS4 × S7/Zk
261.	Kamalakshya Mahatab, IMSc	IMSc	18/10/2013	Nonnegative Solutions of Linear Diophantine Equations-1
262.	Peter Fiebig, FAU, Erlangen-Nuernberg	IMSc	18/10/2013	Modular representations of algebraic groups
263.	Maneesh Thakur, ISI, Delhi	IMSc	22/10/2013	The Kneser-Tits problem
264.	Manjari Bagchi, ICTS, Banagalore	IMSc	23/10/2013	Why Study Pulsars: They Are Awesome
265.	T. Mubeena, IMSc	IMSc	23/10/2013	Twisted conjugacy classes in lattices in semisimple Lie groups
266.	Gyan Prakash, Harish-Chandra Research Institute	IMSc	23/10/2013	Roth's theorem in primes and its generalisation
267.	Manjari Bagchi, ICTS, Bangalore	IMSc	24/10/2013	Binary Radio Pulsars: Prospects and Problems
268.	Maneesh Thakur, ISI Delhi	IMSc	24/10/2013	The Kneser-Tits problem
269.	Gyan Prakash, Harish-Chandra Research Institute	IMSc	24/10/2013	Roth's theorem in primes and its generalisation



270	Arvind Ayyer, IISc, Bengaluru	IMSc	24/10/2013	Markov chains based on Jeu de Taquin
271	Yanjing Wang, Peking University, Beijing, China and ISI-Chennai Centre	IMSc	24/10/2013	An epistemic logical perspective on interpretations of extensive games with imperfect information
272	Arvind Ayyer, IISc, Bangalore	IMSc	25/10/2013	Two Species Semipermeable Exclusion Processes
273	Gyan Prakash, Harish-Chandra Research Institute	IMSc	26/10/2013	Roth's theorem in primes and its generalisation
274	R. Ganesh, IFW, Dresden	IMSc	30/10/2013	Polar Superconductivity in $TiSe_2$
275	G. P. Balakumar, IMSc	IMSc	31/10/2013	Classifying domains in C_n by their automorphism group: a short survey and a case study of domains with abelian automorphism group
276	Arghya Mondal, IMSc	IMSc	01/11/2013	Hirzebruch's Proportionality Principle
277	Anirban Mukhopadhyay, IMSc	IMSc	01/11/2013	Polynomial Freiman-Ruzsa Conjecture
278	Biplob Bhattacharjee, Kavli IPMU, University of Tokyo	IMSc	05/11/2013	Supersymmetry and dark matter search: prospects and challenges
279	Amitabh Virmani, Institute of Physics, Bhubaneswar	IMSc	06/11/2013	Non-supersymmetric Microstates of the MSW System
280	Sayan Bhattacharya, Max Planck Institute, Germany	IMSc	07/11/2013	Price of Anarchy, Auctions and Approximations
281	T. Geetha, IMSc	IMSc	07/11/2013	Schur-Weyl dualities and diagram algebras
282	Anirban Mukhopadhyay, IMSc	IMSc	08/11/2013	Polynomial Freiman-Ruzsa Conjecture



283.	J. Hurtubise, McGill University, Montreal, Canada	IMSc	12/11/2013	Moduli spaces
284.	Amitabh Virmani, Institute of Physics, Bhubaneswar	IMSc	14/11/2013	Inverse Scattering and the Geroch group
285.	Kaushal Verma, IISc, Bangalore	IMSc	14/11/2013	Quadrature domains - a survey
286.	J. Hurtubise, McGill University, Montreal.	IMSc	14/11/2013	Moduli and gauge theory on complex curves
287.	Rukmini Kumar, Vantage Research	IMSc	15/11/2013	Mathematical modeling in pharmaceutical R D
288.	Amritanshu Prasad, IMSc	IMSc	15/11/2013	Frobenius's Characteristic Function Explained
289.	Ms Priya Ramesh	IMSc	15/11/2013	Counseling Psychologist based in Chennai Counselor in Campus
290.	J. Hurtubise, McGill University, Montreal, Canada	IMSc	18/11/2013	Moduli and gauge theory on complex surfaces
291.	J. Hurtubise, McGill University, Montreal, Canada	IMSc	20/11/2013	Moduli and maps of complex curves
292.	Karam Deo Shankhadhar, IMSc	IMSc	21/11/2013	Jacobi forms of weight 2 and restriction map
293.	Christian Schubert, Institute for Physics and Mathematics, Michoacan University, Ciudad Universitaria,	IMSc	21/11/2013	string-inspired calculation techniques in quantum field theory
294.	J. Hurtubise, McGill University, Montreal, Canada	IMSc	22/11/2013	Infinite dimensional aspects of moduli of curves
295.	M. Ram Murty, Queen's University	IMSc	26/11/2013	Indra's Pearls



296	Sayantani Bhattacharyya, Ramkrishna Mission, Vivekananda University	IMSc	27/11/2013	Fluid Dynamics and Gravity
297	Rishi Raj, Dept. of Mathematics, Yale University	IMSc	28/11/2013	Old and New on the Moduli Spaces of Local Systems on Surfaces
298	Sayantari Ghosh, Bose Institute, Kolkata	IMSc	28/11/2013	Bistability in Biology: Signature, Origin and Consequences
299	J. Pasupathy, CHEP, IISC, Bangalore	IMSc	28/11/2013	Bose, Bosons and the Higgs Boson
300	Sayantani Bhattacharyya, Ramkrishna Mission Vivekananda University	IMSc	29/11/2013	Partition Function and Entropy current in Hydrodynamics
301	Amritanshu Prasad, IMSc	IMSc	29/11/2013	Counting Conjugacy Classes of Tuples of Commuting Elements in a Finite Group
302	Himani Sachdeva, TIFR, Mumbai	IMSc	04/12/2013	Phase Transitions in an Open-Boundary Aggregation-Fragmentation Model
303	Hans-Peter Schlickewei. University of Marburg, Germany	IMSc	05/12/2013	The Subspace Theorem in Diophantine Approximation
304	J.PASUPATHY, CHEP, IISc, Bangalore	IMSc	05/12/2013	BCS Theory and the Standard Model of Particle Physics
305	Ashutosh Rai, IMSc, Chennai	IMSc	05/12/2013	Polynomial Kernels for Lambda-extendible Properties Parameterized above the Poljak- Turzk Bound
306	P Sekhar Burada, University of Gottingen, Germany	IMSc	10/12/2013	Passive and active transport
307	Partha Mukhopadhyay, IMSc	IMSc	11/12/2013	Bound configurations, strings and tubular geometry
308	Sanjoy Sarker, University of Alabama	IMSc	11/12/2013	Quantum Lattice (Gauge) order connecting High Tc Superconductivity in Cuprates to Mott insulators



309.	Glen Evenbly, Caltech	IMSc	12/12/2013	Tensor network states beyond the entropic area law
310.	Samit Bhattacharyya, Pennsylvania State University	IMSc	16/12/2013	Oscillations in Biological Populations: Theory and Models
311.	Vijay Ganesh, University of Waterloo, Canada	IMSc	20/12/2013	SAT and SMT solvers for software engineering and security
312.	K B Sinha, JNSCR Bangaluru	IMSc	23/12/2013	Trace formula in two variables
313.	K. B. Sinha, JNCASR, Bangaluru	IMSc	26/12/2013	Stopped CCR-flows and Isometric Cocycles
314.	Sinai Robins, Nanyang Technological University	IMSc	01/01/2014	Cone theta functions, volumes of spherical polytopes, and their relations to classical theta functions
315.	Hans van Ditmarsch, LORIA (CNRS - University of Lorraine) and IMSc (associate)	IMSc	02/01/2014	Refinement modal logic
316.	J. Maharana, Institute of Physics, Bhubaneswar	IMSc	03/01/2014	T-duality and scattering of stringy states
317.	Areejit Samal, ICTP, Trieste, Italy	IMSc	03/01/2014	Reconstruction and systems analysis of plant cell wall deconstruction network in filamentous fungus
318.	Ashivni Shekhawat Material Science and Engineering, UC Berkeley.	IMSc	06/01/2014	What has fracture got to do with magnets and the liquid-vapor critical point?
319.	Martin Bojowald, Institute for Gravitation and the Cosmos, Univ. of Penn., USA	IMSc	07/01/2014	Effective space (-time) in canonical quantum gravity
320.	Ram Gopal Vishwakarma, Universidad Autnoma de Zacatecas, Mexico	IMSc	08/01/2014	Introduction of Tik: Einsteins Real Biggest Blunder?
321.	Yuri Bilu, University of Bordeaux	IMSc	09/01/2014	Effective methods in Diophantine Analysis



322	Supravat Dey, Universita' di Roma La Sapienza,	IMSc	10/01/2014	Short range interaction from long-range correlation in flocks of birds
323	Dhriti Ranjan Dolai, IMSc	IMSc	10/01/2014	Spectral statistic for Anderson model with decaying random potential
324	Amritanshu Prasad, IMSc	IMSc	10/01/2014	Abacus Proofs of Schur Function Identities (Following Nicholas A. Loehr)
325	Rajsekar Manokaran, KTH Sweden	IMSc	13/01/2014	Invariance Principle and Unique Games
326	Yuri Bilu, University of Bordeaux	IMSc	14/01/2014	Effective methods in Diophantine Analysis
327	Professor Barbara Fantechi, CMI, VISITOR	IMSc	14/01/2014	An introduction to Intersection Theory
328	Rajsekar Manokaran KTH Sweden	IMSc	15/01/2014	Approximation hardness using Unique Games
329	Rohit Parikh, City University of New York, USA.	IMSc	17/01/2014	Regular Sets, Well Partial Orders and Levels of Knowledge
330	Anil Kumar C P, IMSc	IMSc	17/01/2014	Characterization of Rational Triangles in the plane
331	Arijeet Samal	IMSc	17/01/2014	Metabolic Networks
332	S. Sundar, CMI	IMSc	21/01/2014	Groupoids associated to Semigroup actions
333	Shivam, St Xevier's School Ahmedabad	IMSc	21/01/2014	Computing some integrals
334	S. Srinivasa Rao	IMSc	21/01/2014	Alphabet friendly FM index
335	S. Sundar, CMI	IMSc	23/01/2014	Groupoids associated to Semigroup actions (Reloaded)



336	Ben Elias, Massachusetts Institute of Technology	IMSc	23/01/2014	Categorical actions of Coxeter groups and braid groups
337	Mansi Dhuria, IIT Roorkee	IMSc	24/01/2014	Aspects of D3/D7 mu-split Supersymmetry
338	Yuri Bilu, University of Bordeaux	IMSc	24/01/2014	Effective methods in Diophantine Analysis
339	Arjun Menon, University of Oregon	IMSc	24/01/2014	SUSY in light of the 8 TeV LHC
340	Amritanshu Prasad, IMSc	IMSc	24/01/2014	Character Tables of Alternating Groups
341	Prateep Chakraborty, IMSc	IMSc	24/01/2014	Stable Homotopy and Spectra
342	Samir Mathur, Ohio State University	IMSc	27/01/2014	Nag Memorial Lecture: technical seminar 1/3
343	Suratna Das, Astronomy and Astrophysics Division, TIFR, Mumbai	IMSc	27/01/2014	CSL as a plausible mechanism for quantum to classical transition of primordial perturbations
344	Samir Mathur, Ohio State University	IMSc	28/01/2014	Nag Memorial Lecture: technical seminar 2/3
345	S. Sundar, CMI	IMSc	28/01/2014	Groupoids associated to Semigroup actions (Revolutions)
346	Samir Mathur, Ohio State University	IMSc	29/01/2014	Nag Memorial Lecture: technical seminar 3/3
347	Prof. Yuri Bilu, Universit de Bordeaux	IMSc	29/01/2014	Effective methods in Diophantine Analysis
348	Ueli Grossniklaus, Institute of Plant Biology, University of Zurich	IMSc	29/01/2014	Theoretical and Experimental Approaches to Study Cell Specification in the Embryo Sac of Arabidopsis thaliana
349	Arjun Menon, University of Oregon	IMSc	30/01/2014	Searching for neutral Higgs bosons in non-standard channels



350.	Prof. Samir Mathur, Ohio-State University	IMSc	30/01/2014	Informal discussion on fuzzballs
351.	Nivedita Chatterjee, Vision Research Foundation, Chennai	IMSc	30/01/2014	Neuroscience (part of Biology-2 course of Comp Bio)
352.	Samir Mathur, Ohio State University	IMSc	31/01/2014	Nag Memorial Lecture
353.	Ben Elias, Massachussets Institute of Technology	IMSc	31/01/2014	Soergel bimodules and Kazhdan-Lusztig theory
354.	Ben Elias, Massachussets Institute of Technology	IMSc	31/01/2014	The new homological algebra: p-complexes and categorification at roots of unity
355.	Arijit Saha, University of Basel, Klingelbergstrasse 82, Switzerland	IMSc	03/02/2014	Transport signatures of Fractional Fermions in Nanowires
356.	Ben Elias, Massachussets Insitute of Technology	IMSc	03/02/2014	Soergel bimodules and Kazhdan-Lusztig theory
357.	Yuri Bilu, University of Bordeaux	IMSc	04/02/2014	Effective methods in Diophantine Analysis
358.	Ian Munro, University of Waterloo, Canada	IMSc	04/02/2014	Succinct Data Structures for representing equivalence classes
359.	Sudhakar Yarlagadda, SINP, Kolkata	IMSc	04/02/2014	An analysis of the extremely anisotropic next-nearest-neighbour Heisenberg Model
360.	Sandipan De, IMSc	IMSc	04/02/2014	Crossed Products of Hopf algebras, the Drinfeld Double construction and a Duality Theorem
361.	Rahul Sinha, IMSc	IMSc	05/02/2014	New Physics effects and Hadronic form factor uncertainties in $B \rightarrow K\ell\ell$
362.	B. Ravinder, IMSc	IMSc	07/02/2014	Current algebras and their Representations
363.	Prabwal Jyoti Phukon, IIT, Kanpur	IMSc	10/02/2014	R charged black holes and holographic optics



364	Sudipto Paul Chowdhary, IMSc	IMSc	11/02/2014	BCS Instability and Finite Temperature Corrections to Tachyon Mass in Intersecting D1-Branes
365	Swastik Bhattacharya, IMSc	IMSc	12/02/2014	Einstein Equation from Thermodynamics: A Generalisation
366	Mukund Thattai, NCBS Bangalore	IMSc	12/02/2014	The watchmaker's apprentice: building a synthetic genetic oscillator with parts borrowed from nature
367	G Arunkumar, IMSc	IMSc	12/02/2014	The Weyl Character Formula
368	Somdeb Ghose, IMSc	IMSc	14/02/2014	Population fluctuations, non-equilibrium flows and instabilities in some model systems.
369	M. Muthukumar, University of Massachusetts, Amherst	IMSc	17/02/2014	Menagerie of Viruses: Organizing Principles of Virus Assembly
370	Patrick Nicholson, Max Planck Institute, Germany	IMSc	17/02/2014	Deterministic schemes for membership in the bitprobe model
371	Denis Benois, University of Bordeaux	IMSc	18/02/2014	Iwasawa theory
372	Saurabh Gupta, IMSc	IMSc	18/02/2014	High Scale Mixing Unification for Dirac Neutrinos
373	Yash Raj Shrestha, University of Saarland, Germany	IMSc	18/02/2014	The complexity of disjoint Pi-vertex deletion
374	G. Arun Kumar, IMSc	IMSc	19/02/2014	The Weyl Character Formula
375	Santosh Ansumali, JNCASR	IMSc	21/02/2014	Lattice Based Computing: Role of Symmetry and Structures
376	Kamalakhya Mahatab, IMSc	IMSc	21/02/2014	Rough Numbers in Arithmetic Progressions
377	Biswajit Paul, SNBNCBS, Kolkata	IMSc	24/02/2014	Gauge Symmetries In higher derivative theories



378	Mridupawan Deka, BLTP, Joint Institute of Nuclear Research,	IMSc	25/02/2014	"Proton Spin Crisis" and A Lattice Study of Quark Gluon Angular Momenta Contributions
379	Zodinmawia, Indian Institute of Technology, Mumbai	IMSc	26/02/2014	Knot invariants from Chern-Simons theory and Knot homology
380	Ramray Bhat, Life Sciences Division, Lawrence Berkeley National Laboratory	IMSc	26/02/2014	Key themes on the development and evolution of mesenchymal morphogenesis and patterning
381	Can Baskent, LORIA, Nancy, France	IMSc	27/02/2014	Game semantics and non-classical logics
382	Fabien Schang, Moscow State University, Russia	IMSc	27/02/2014	A logic for Tetris
383	Indira Mishra, IMSc	IMSc	27/02/2014	C-semigroups and almost periodic solution
384	Abhishek Iyer, IISc	IMSc	28/02/2014	How to hide lepton number violation
385	Ramkarthik Seshadri, IIT-Madras	IMSc	28/02/2014	Two studies on Quantum Entanglement: Optimal Mixtures and Dimerization in the Majumdar-Ghosh Model
386	Uday Bhaskar Sharma, IMSc	IMSc	28/02/2014	Counting Simultaneous Similarity Classes of Commuting Matrix Tuples
387	Varuni Prabhakar, PhD, New York University	IMSc	03/03/2014	The dynamics of age in populations of <i>Saccharomyces cerevisiae</i>
388	Ravin Bhatt, Princeton University and Institute of Advanced Study,	IMSc	04/03/2014	The Anderson Model of Localization: Has the fat lady sung yet?
389	Vikas Bansal, Pacific Northwest National Lab, US	IMSc	06/03/2014	Prospects of Leptoquark discovery with ATLAS at the LHC
390	Shreedevi Masuti, IMSc	IMSc	07/03/2014	Rees Theorem
391	Chandrajit Lahiri, IMSc, Chennai	IMSc	07/03/2014	Disease Complexity - A Bird's Eye View



392	Uday Bhaskar Sharma, IMSc	IMSc	07/03/2014	Counting Conjugacy Classes of Tuples of Commuting Elements in a Finite Group
393	D. Yogeswaran, Technion, Israel	IMSc	10/03/2014	Central limit theorems for some random simplicial complexes
394	R. Srinivasan, CMI	IMSc	13/03/2014	Many CCR flows
395	Ronny Thomale, Institut fr Theoretische Physik 1, Julius-Maximilians Universitt Wrzburg, Germany	IMSc	17/03/2014	The Quest of the Kagome Hubbard Model
396	Preeda Patcharamaneepakorn, JNU	IMSc	18/03/2014	Travelling Front of a Decaying Brane
397	Leelavati Narlikar, National Chemical Laboratory, Pune	IMSc	19/03/2014	Characterizing the heterogeneity in high-throughput sequencing data to understand transcriptional regulation
398	S. Kalyana Rama, IMSc	IMSc	19/03/2014	Stars in M theory (made up of intersecting branes)
399	Saibal Ganguli, IMSc	IMSc	20/03/2014	Mckay correspondence and almost complex structures on quasitoric orbifolds
400	Pierre Fima, University of Paris	IMSc	21/03/2014	Graphs of Quantum Groups and K-Amenability
401	L. Sriramkumar, IIT Madras	IMSc	21/03/2014	On the detection of the imprints of primordial gravitational waves on the CMB by BICEP2
402	Pierre Fima, University of Paris	IMSc	24/03/2014	Graphs of Quantum Groups and K-Amenability
403	Vijay Ravikumar, TIFR	IMSc	24/03/2014	The Cohomology Ring of the Complex Grassmannian
404	Pierre Fima, University of Paris	IMSc	25/03/2014	Graphs of Quantum Groups and K-Amenability



405	Vijay Ravikumar, TIFR	IMSc	25/03/2014	Triple Intersection Formulas for Isotropic Grassmannians
406	Pierre Fima, University of Paris	IMSc	26/03/2014	Graphs of Quantum Groups and K-Amenability
407	A.P. Dimri, JNU, New Delhi	IMSc	27/03/2014	Role of the Himalaya in defining Indian Weather and Climate



Academic Report 2013-14



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)

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

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. M.K.Sanyal Director, SINP	Member
Prof. R. A. Badwe Director, TMC	Member
Prof. R. Balasubramanian Director, IMSc	Member
Prof. M. Barma Director, TIFR	Member
Prof. T.K. Chandrashekar /V. Chandrashekar Director, NISER	Member
Prof. J. K. Bhattacharjee Director, HRI	Member
Prof. A.M. Jayannabar/ 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. C.S.Sundar
Indira Gandhi Centre for Atomic Research
3. Prof. S Ganesh
Institute of Plasma Research
4. Prof. Ajit Srivastava
Institute of Physics
5. Prof. P.K.Gupta
Raja Ramanna Centre for Advanced Technology
6. Prof. Pinaki Majumdar
Harish-Chandra Research Institute
7. Prof. P. Mitra
Saha Institute of Nuclear Physics
8. Prof. Ramesh Anishetty
Institute of Mathematical Sciences
9. Prof. B.N.Jagtap
Bhabha Atomic Research Centre
10. Prof. S L Chaplot
Bhabha Atomic Research Centre

Chemical Sciences

1. Prof. K. L. Ramakumar **Convener**
Bhabha Atomic Research Centre
2. Prof. A. V. R. Reddy
Bhabha Atomic Research Centre
3. Prof. A. Goswami
Bhabha Atomic Research Centre
4. Prof. Swapan Ghosh (upto 30.09.2013)
Bhabha Atomic Research Centre
5. Prof. V. Ganesan
Indira Gandhi Centre for Atomic Research
6. Prof. K. Nagarajan
Indira Gandhi Centre for Atomic Research
7. Prof. V.K Jain
Bhabha Atomic Research Centre
8. Prof. A. Srinivasan
Head, School of Chemistry, NISER (IOP)
9. Prof. S. Chattopadhyaya
Bhabha Atomic Research Centre



Life Sciences

1. Prof. S.K. Apte
Bhabha Atomic Research Centre
2. Prof. (Mrs.) S. Chiplunkar
Advanced Centre for Treatment, Research
& Education in Cancer (ACTREC)
3. Prof. Rita Mulherkar
Advanced Centre for Treatment, Research
& Education in Cancer (ACTREC)
4. Prof. S. P Kale
Bhabha Atomic Research Centre
5. Prof. J.R. Bandekar
Bhabha Atomic Research Centre
6. Prof. A.K.Sharma
Bhabha Atomic Research Centre
7. Prof. B. J. Rao
Tata Institute of Fundamental Research
8. Prof. Dipak Dasgupta
Saha Institute of Nuclear Physics

Convener

Engineering Sciences

1. Prof. P.K. Vijayan
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. Kamachi Mudali
Indira Gandhi Centre for Atomic Research
8. Prof. Kallol Roy
Bhabha Atomic Research Centre
9. Prof. P. V. Varde
Bhabha Atomic Research Centre
10. Prof. D. N. Badodkar
Bhabha Atomic Research Centre

Convener



Mathematical Sciences

1. Prof. R. Ramanujam
Institute of Mathematical Sciences
2. Prof. Amritanshu Prasad
Institute of Mathematical Sciences
3. Prof. B. Ramakrishnan
Harish-Chandra Research Institute
4. Prof. C.S.Sunder
Institute of Mathematical Sciences
5. Prof. N. Raghavendra
Harish-Chandra Research Institute
6. Prof. R.C.Cowsik
Mumbai University
7. Prof. Murali Srinivasan
Indian Institute of Technology-Bombay
8. Prof. Madhavan Mukund
Chennai Mathematics Institute
9. Prof. Muruganandam
NISER

Convener

Strategic Studies

1. Prof. K.L. Ramakumar
Bhabha Atomic Research Centre
2. Dr. A.K. Kohli
Board of Radiation and Isotope Technology
3. Prof. R. B. Grover
Director HBNI
4. Dr. B. B. Singh
Ex-BARC and Scientific Advisor, High Court Mumbai
5. Prof. Rangan Banerjee
Indian Institute of Technology-Bombay
6. Prof. M. Sai Baba
Indira Gandhi Centre for Atomic Research
7. Dr. J. Kumar
Legal Adviser, DAE

Convener



Health Sciences

- | | |
|---|-----------------|
| 1. Prof. K. S. Sharma
Tata Memorial Centre, Mumbai | Convener |
| 2. Prof. D. D. Deshpande
Tata Memorial Hospital, Mumbai | |
| 3. Prof. K. B. Sainis
Bhabha Atomic Research Centre, Mumbai | |
| 4. Prof. S. K. Srivastava
Tata Memorial Hospital, Mumbai | |
| 5. Dr. H. B. Tongaonkar/ P.S. Yadav
Tata Memorial Hospital, Mumbai | |
| 6. Dr. S. B. Banavali
Tata Memorial Hospital | |
| 7. Prof. N. A. Jambekar
Tata Memorial Hospital, Mumbai | |
| 8. Prof. Shubhangi Parkar
KEM Hospital, Mumbai | |
| 9. Prof. Avinash Supe
LTMG Hospital, Mumbai | |
| 10. Prof. M. G. R. Rajan
Radiation Medicine Centre, Mumbai | |

Officers of the Institute

Academic

Prof. R.B. Grover	Director
Prof. B.K. Dutta	Dean
Prof. D. K. Maity	Associate Dean (w.e.f. 01.08.2013)
Dr. R. P. Patel	Associate Dean (up to 31.07.2013)

Administrative and Accounts

Shri A. Ramaiah	Finance Officer (up to 31.07.2013)
Shri Himanshu Shankar	Finance Officer (w.e.f. 01.08.2013)
Ms. B. Lata	Administrative Officer
Shri Yellapan / H K Pal	Accounts 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. B. N. Jagatap	Physical Sciences
Prof. Swapan K. Ghosh	Chemical Sciences (upto 30.09.2013)
Prof. B. S. Tomar	Chemical Sciences (w.e.f. 01.10.2013)

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



BARC Standing Committees

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.) Sharmila Banerjee	Member
5. Dr. B. K. Sapra	Member
6. Dr. M. S. Kulkarni	Member
7. Dr. Biriagalaxmi 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)

RRCAT Standing Committee

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



IGCAR Standing Committees

Physical Sciences

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

Chemical Sciences

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

Engineering Sciences

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



VECC Standing Committee

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

IPR Standing Committee

- | | |
|-----------------------|----------|
| 1. 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 |



Academic Report 2013-14



Annex 3

Faculty List (01 April 2013 to 31 March 2014)



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. Alok Kumar Samanta
8. Anil Kumar Pabby
9. Arya Ashok Kumar
10. Aswal D. K.
11. Bandyopadhyay Tusar
12. Banerjee A. (Ms.)
13. Banerjee Sharmila (Ms.)
14. Bharadwa. S.R. (Ms.)
15. Bhardwaj Y.K.
16. Bhasikuttan A.C.
17. Bindal R.C.
18. Chakraborty Sudipta (Ms.)
19. Chandrakumar K.R.S.
20. Chatterjee Suchandra (Ms.)
21. Chattopadhyay A.
22. Chattopadhyay Subrata
23. Chaudhury Niharendu
24. Chowdhury D.P.
25. Das D.
26. Das Tapas
27. Das Tomi Nath
28. Dash Smruti (Ms.)
29. Dash Ashutosh
30. Deo Mukul Narayan
31. Dey Ghasiram
32. Dey Sandip
33. Dhanya S.
34. Dutt G.B.
35. Dutta Dimple (Ms.)
36. Ganguly R.
37. Ghanty Tapan Kumar
38. Ghosh Asim Kumar
39. Ghosh Hirendra Nath
40. Ghosh Subir Kumar
41. Ghosh Sunil K.
42. Ghosh Swapan K.
43. Goswami Madhumita (Ms.)
44. Goswami A.
45. Gupta Vinita Grover (Ms.)
46. Hassan P.A.
47. Jain V.K.
48. Jha S.K.
49. Kadam R.M.
50. Kannan S.
51. Kapoor Sudhir
52. Kaushik C.P.
53. Korde Aruna (Ms.)
54. Krishnamurthy Nagaiyar
55. Kshirsagar R.J.
56. Kumar Sangita D. (Ms.)
57. Kumar Virendra
58. Kumar Awadhesh
59. Kumar Sanjukta A. (Ms.)
60. Maity Dilip K.
61. Majumder C.
62. Manmohan Kumar
63. Meera Venkatesh (Ms.)
64. Mishra N.L.
65. Mishra R.
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21. Chaturvedi P.
22. Chaukar D.A.
23. Chavan Preeti
24. Chinnaswamy G.R.
25. Chopra Supriya
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27. D'cruz A.K.
28. Deodhar K.K.
29. Deodhar J.K. (Ms.)
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31. Desai S.M.
32. Desai P.D. (Ms.)
33. Desai S.B. (Ms.)
34. Deshmukh A.D. (Ms.)
35. Dholam K.P. (Ms.)
36. Divatia J.V.
37. Doctor J.R.
38. Engineer R. (Ms.)
39. Gehdoo R.P.
40. Ghosh Jaya
41. Goel M.
42. Gota Vikram
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48. Jain P.
49. Jain Hasmukh
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62. Kerkar R.A.
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67. Kulkarni S.S.
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71. Laskar S.S.
72. Mahajan A.
73. Mahantshetty U.M.
74. Maheshwari A. (Ms.)
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82. Muckaden M.A. (Ms.)
83. Murthy Vedang
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86. Nair N.S. (Ms.)
87. Nair Sudhir V.
88. Narula Gaurav
89. Noronha V.M.
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98. Patil V.P. (Ms.)
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102. Poojary Minal
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104. Prakash Gagan
105. Pramesh C.S.
106. Prasad Maya (Ms.)
107. Purandare N.C.



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120. Sahay Ayushi (Ms.)
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131. Shetmahajan xM.G. (Ms.)
132. Shetty N.S.
133. Shetty N.S.
134. Shrikhande S.V.
135. Shrivastava S.K.
136. Solanki S.L.
137. Sridhar Epari
138. Subramanian P.G.
139. Surappa S.T.
140. Tandon S.P.
141. Tembhare Prashant
142. Tendulkar A.A. (Ms.)
143. Thakur M.H. (Ms.)
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145. Trivedi Bhakti
146. Vora Tushar S.
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3. Bhattacharyya Dibyendu
4. Bose Kakoli
5. Chiplunkar S.V. (Ms.)
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7. De Abhijit
8. Deodhar Kedar K.
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11. Dutt Shilpee (Ms.)
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13. Gota Vikram
14. Govekar Rukmini (Ms.)
15. Gude Rajiv P.
16. Gupta Sanjay
17. Gupta Tejpal
18. Joseph Ms. Lebana J.
19. Joshi Narendra N.
20. Kadam P.S. Amare (Ms.)
21. Kalraiya Rajiv D.
22. Krishna C.M.
23. Kumar Chandan
24. Laskar Sarbani Ghosh (Ms.)
25. Mahantshetty Umesh M.
26. Mahimkar Manoj B.
27. Mallath M.K.
28. Myatra Sheila N. (Ms.)
29. Naik Nishigandha R. (Ms.)
30. Rai Rekha (Ms.)
31. Ramadwar Mukta (Ms.)
32. Ramani S.K.
33. Ray Pritha
34. Shirsat Neelam Vishwanath (Ms.)
35. Teni Tanuja R. (Ms.)
36. Thakur M.H.
37. Vaidya Milind M.
38. Varma Ashok K.
39. Venkatraman Prasanna
40. Waghmare Sanjeev K.

Life Sciences

1. Arya Supreeta (Ms.)

Physical Sciences

1. Deshpande D.D



Academic Report 2013-14



Annex 4

Abstracts of Ph.D. Theses (April 1, 2013 to March 31, 2014)



Name : **Sanjay Kumar**
Enrolment No. : CHEM01200904010
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Studies on Hydrogen Interaction with Vanadium and Vanadium-Aluminium Alloys

Abstract

The present investigation begins with certain aspects of the process development of vanadium, its alloys with Cr, Ti & Al and V-LaNi₅ composite with reference to hydrogen solubility and sorption kinetics study. Efforts were made for the synthesis of vanadium metal and its alloys, V-Al, V-Ti, V-Cr and V-Ti-Cr by aluminothermy process followed by electron beam melting. The composite LaNi₅ - 80wt% V was prepared by vacuum arc melting techniques using pure LaNi₅ and vanadium. The experimentation with process parameters for the improved percentage yield of aluminothermy was achieved. The development of Sieverts apparatus with a high precision thermobalance was done to study the equilibrium hydrogen solubility and sorption kinetics of metal hydrogen systems. Hydrogen solubility and the hydrogen sorption kinetic results of the above mentioned materials would be explained by various correlations such as Fermi energy theory, density functional theory, mechanical effects, grain refinement and catalytic properties of additives.

Chapter 1 describes a brief introduction of the current hydrogen storage issues and the mechanism of the hydrogen interaction of the solid materials. The brief history of vanadium metals and its importance in the development as a structural and functional applications in advanced energy systems have been illustrated. The outline of the thesis work is also presented in this chapter. Chapter 2 deals with the review of recent literature on vanadium based hydrogen storage and permeation systems. The role of vanadium as grain refinement and Laves phase formation in the various alloys and intermetallic as a candidate hydrogen storage materials has been illustrated in detail. Chapters 3 describe the materials and methods used in the investigation. Most of the materials have been synthesized by aluminothermy using respective oxides followed by electron beam melting. Materials were also synthesized by vacuum arc melting using pure components for the comparative study. The details of the modified Sieverts apparatus specially developed for this work was described. All the modern instrumental techniques which have been used in the present investigation such as XRD, SEM-EDS, TEM, Ball Milling, DSC, AES, ICPAES and XPS have been presented in detail. The Chapter 4 consists of four parts. The first subsection is based on the results of materials synthesis by aluminothermy process. Thermodynamic feasibility of the aluminothermy reduction of Cr₂O₃, TiO₂ and V₂O₅ has been computed and found that though the aluminothermy reduction enthalpy of TiO₂ is not sufficient to sustain the reaction: its reduction is possible along with Cr₂O₃ and V₂O₅. The reduction Cr₂O₃ and V₂O₅ is highly exothermic which is sufficient to make-up the shortfall of enthalpy of TiO₂ reduction by aluminum. Loading of Ti into the vanadium matrix by aluminothermy process using their respective oxides is an innovative outcome of the investigation. It was found that use of heat booster and slag fluidizers such as CaF₂, CaSiO₃ and CaO in aluminothermy process sufficiently improves the percentage yield of the process. Second subsection explain the hydrogen solubility behavior of hydrogen of vanadium. The hydrogen solubility of vanadium is accompanied substantial lattice expansion of vanadium. The hydrogen solubility decreases with aluminum. The steps involved during the de-hydriding of VH₂ have been studied using thermogravimetric (TG) and thermal analysis (DSC) technique and presented in the third subsection of this chapter. It was found that aluminum sufficiently reduce the thermal stability of vanadium hydride. Thermodynamic parameters such as enthalpy and enthalpy of vanadium-hydrogen



solid solution has been described in the subsection fourth of this chapter. The effects of aluminum on the thermodynamic parameters have been studied and correlated on the basis of Fermi energy theory. The kinetics of hydrogen absorption of V-Al alloys, V-Ti-Cr and V-LaNi₅ composite have been investigated and presented in the same subsection. It was found that the hydrogen absorption mechanism varied with the temperature and incubation time. The activation energy of hydrogen absorption of vanadium increases with aluminum. Hydrogen absorption kinetics of LaNi₅-V composite has also been studied. Lattice expansion of LaNi₅ in the composite has been observed in X-ray analysis which indicates the solid solution formation. The hydrogen absorption capacity and absorption kinetics of the composite showed improvement as compared to LaNi₅. The improved Kinetics of the composite has been related to change in lattices parameter, Fermi energy level and catalytic property of vanadium. The effects of vanadium on pulverization of composite after 20 hydriding-dehydriding cycle have also been studied using scanning electron microscopy and found that the integrity of the composite had shown improvements. In Chapter 5, a summary of the thesis has been given. Possible future work on the basis of present thesis has also described in this chapter.

The candidate has done extensive and good quality work on materials synthesis and hydrogen interaction of these materials. The investigation is direct focuses on the issues related to hydrogen storage materials and was led good quality international publications. Therefore, I strongly recommend that the thesis be accepted for the award of degree of Ph.D to Shri Sanjay Kumar.

Publications

Publications in International Journals from the Ph.D work

1. Sanjay Kumar and N Krishnamurthy Synthesis of V-Ti-Cr alloys by aluminothermy co-reduction of its oxide *International Journal of Processing and Application of Ceramics* 2011;5(4):181-6.
2. Sanjay Kumar, M Taxak, N Krishnamurthy, A K Suri and GP Tiwari Terminal solid solubility of hydrogen in V-Al solid solution *International Journal of Refractory Metals and Hard Materials* 2012; 31: 76-81
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4. Sanjay Kumar and N Krishnamurthy Variation of activation energy of hydrogen absorption of vanadium as a function of Al *International Journal of Hydrogen Energy*, 2012; 37(18) 13,429-36.
5. Sanjay Kumar and N Krishnamurthy Effects of aluminum on solubility and β phase stability of vanadium-hydrogen system *International Journal of Refractory Metals and Hard Materials* 2012; 35: 191-5.
6. Sanjay Kumar, M Taxak and N Krishnamurthy Hydrogen absorption kinetics of V-Al alloy *Journal of Thermal Analysis and Calorimetry* 2012; DOI: 10.1007/s10973-012-2558-1.
7. Sanjay Kumar M Taxak and N Krishnamurthy Synthesis and hydrogen absorption in V-Ti-Cr alloy *Journal of Thermal Analysis and Calorimetry* 2012; DOI 10.1007/s10973-012-2643-5.
8. Sanjay Kumar and N Krishnamurthy Effects of Aluminum on standard enthalpy and entropy of vanadium-hydrogen solid solution *Int J Hydrogen Energy* 2013, HE-D-13-00850, under review.
9. Sanjay Kumar, A Tirpude, M Taxak and N Krishnamurthy Hydrogen absorption kinetics in ball milled V+ 80wt% LaNi₅ composite *Journal of Alloys and Compounds* 2012, doi: 10.1016/j.jallcom.2013.03.001.



10. Sanjay Kumar and N. Krishnamurthy Development of vanadium based hydrogen storage materials: a review *Progress in Materials Science 2012; to be submitted.*
11. Sanjay Kumar, M Taxak and N Krishnamurthy Solid state hydrogen storage methods: theories and applications *Indian Thermal Society of India, ITAS 2012, Invited paper to be submitted xii*

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1. Sanjay Kumar, M Taxak and N Krishnamurthy. Hydrogen absorption kinetics in V-Al alloys. Proceeding of the 18th International Symposium on Thermal Analysis, Editors: R Agrawal, L Varshney, YK Bhardwaj, RA Jat, S K Rakshit, K L Ramkumar 2012; 333-5.
2. Sanjay Kumar, M Taxak and N Krishnamurthy. Synthesis and Hydrogen absorption Kinetics of V₄Cr₄Ti alloys. Proceeding of the 18th International Symposium on Thermal Analysis, Editors R. Agrawal, L Varshney, YK Bhardwaj, RA Jat, SK Rakshit, KL Ramkumar 2012; 315-7.
3. Sanjay Kumar, M Taxak and N. Krishnamurthy. Solid solubility of hydrogen in V-Ti-Cr-Al alloys synthesize by aluminothermy. 49th NMD and 65th ATM 13-16 Nov 2011 Hyderabad India Editors Dr. Amol A Gokhale and Dr. Shrikant V Joshi; p 63
4. Sanjay Kumar, M Taxak and N Krishnamurthy. Interaction of hydrogen with pure vanadium. 49th NMD and 65th ATM 13-16 Nov 2011 Hyderabad India Editors Dr. Amol A Gokhale and Dr. Shrikant V Joshi. p 89
5. M Taxak, Sanjay Kumar, N Krishnamurthy, A K Suri and G P Tiwari. Effect of aluminum on the equilibrium solubility of hydrogen in vanadium. Proceedings of 3rd International Symposium on Materials Chemistry (2010) Mumbai India Editor Dr. R K Vatsa; p 113.
6. Sanjay Kumar, A Awasthi, R.N. Singh and N Krishnamurthy. Solid Solubility in Vanadium-Aluminum alloys. HEM 2009, Mumbai, India , Editor Dr. R.N Singh; p 46
7. N. Krishnamurthy, Sanjay Kumar, A. Awasthi. Preparation of binary alloys of refractory metals by co-reduction: Group V Metals alloy. Vol.1 RM30/1-RM30/10, 17th Plansee Seminar Proceeding, Plansee Group, Austria2009; 1-10.
8. Sanjay Kumar, M Taxak and N Krishnamurthy. Hydrogen absorption kinetics in ball milled V+80wt.% LaNi₅ composite, International Symposium on Metal-Hydrogen Systems-Fundamentals and Applications- 21-26 October, 2012 Kyoto, Japan.



Name : **M. R. Gonal**
Enrolment No. : CHEM01200604026
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Preparation of Bulk High Temperature Super Conductors by Textured Growth Techniques, and their Characterization

Abstract

The main focus of this thesis is to develop viable technologies to process the brittle ceramic High Temperature Superconducting (HTSC) material $\text{YBa}_2\text{Cu}_3\text{O}_{7-8}$ (Y-123) into commercially usable forms. To achieve this objective the efforts were concentrated in following areas such as synthesizing powders through different routes, detailed study of sintering and phase conversion process. The powders were well characterized by XRD for phase analysis and laser particle size analyzer for particle size measurements.

Top Seeded Melt-texture (TSMTG) technique was used and for fabrication of hollow cylinder and plates. Y_2BaCuO_5 (Y-211) powder was synthesized using two different routes resulting in different particle sizes to the polycrystalline $\text{YBa}_2\text{Cu}_3\text{O}_{7-8}$ superconductor using MgO as seed crystal created an essentially highly dense structure consisting of cm long, plates shaped crystals preferably aligned parallel to the a-b plane.

The TSMTG components were characterized using XRD, SEM, TEM, OIM, EPMA, for trapped magnetic field. Levitation force and J_c . Texturing were studied by XRD and OIM. OIM orientation is in corroboration with XRD analysis which revealed that all the peaks correspond to 001 oriented plane. OIM graph also showed the quantity and particle size of Y-123 and Y-211 phases. Electron Probe Micro-Analyzer(EPMA) image and corresponding elemental mapping show particle size distribution of Y-211 phase in the matrix of YBCO. These experiments also reveal the line profile of the variation of individual elements from matrix of Y-123 (superconducting) and Y-211 (non-superconducting) phases. Trapped magnetic field levitation force measured by indigenously developed system. The maximum trapped field values for TSMTG plate prepared by solid state route and for TSMTG sample prepared from nitrate decomposition route were 0-200 gauss and 0-800 gauss, respectively. Levitation force measured at 1 mm distance from magnet of TSMTG plate prepared by solid state route show force of 8 n and whereas in TSMTG sample prepared by Y-211 synthesized by nitrate decomposition route show force of 28 N. J_c were measured at Budapest University of technology and Economics (BUTE), Hungary. Average J_c values of TSMTG hollow cylinder at 77 K of 3500-4000 A/cm in zero field (compared to 500-1 A/cm² in sintered bodies).

The new micro structure, which completely replaces the previous granular and random structure in the sintered bodies, exhibits improved superconducting properties. The remarkable improvement in J_c , levitation force, and trapped magnetic field is attributed to the combined effects of graded Y-211 particles, compaction, thermal cycle, alignment of crystals, formation of cleaner grain boundaries. The J_c measured in other TSMTG samples generated using Pt, ceria added additives were found to be lower as compared to that from Y-211 addition.



Publications

Journal

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2. Bulk High Temperature Superconductors Prepared by Melt Textured GrowthTechnique- Effect of Y2BaCuO5 Particle Size M. R. Gonal, R.C. Hubli and A.K. Tyagi AIP Conf. Proc. 1349, (2011) 833-834
3. Study of Superconducting Properties in Melt Textured YBCO samples M. R. Gonal, K.G.Bhushan, S Ramanathan, R.C. Hubli, A.K. Tyagi, and G.P.Kothiyal AIP Conf. Proc. 1447, pp. 911-912
4. The Effect of Addition of Y-211 with two Different Particle Sizes on the Properties of Melt Processed YBa₂Cu₃O_{7-δ} (YBCO) Bulk Superconductors M. R. Gonal, R.C. Hubli, A.K.Suri, A.K. Tyagi, Atila Gyore and Istvan Vajda IEEE transactions on Applied Superconductivity (Communicated)

Symposium

1. Characterisation of Bulk High Temperature Superconductors Prepared by Melt Textured Growth Technique M. R. Gonal, R.C. Hubli and A.K. Tyagi† *Proceedings of the 54th DAE Solid State Physics Symposium (2009)*



Name : **Raja Kishora Lenka**
Enrolment No. : CHEM01200604025
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Nano Electroceramics for Intermediate Temperature Solid Oxide Fuel Cell

Abstract

My doctoral thesis was aimed towards development of nano-electroceramics for IT-SOFC application. Gadolinia doped ceria has been chosen as the electrolyte material. Ni-GDC and Ba-doped GdCoO₃ have been considered as the anode and cathode materials, respectively. Gadolinia doped ceria (12 mol%) powder was synthesized by combustion route using different fuels. The characteristics of the processes have been studied by thermal analysis of gel precursor. The processes have been analyzed through thermodynamic calculation. Physical properties of powders prepared through different route were characterized. Based on the characteristics of the synthesized GDC powder metal nitrate - citric acid gel combustion route was chosen for the preparation of powder. In order to study the effect of dopant concentration on the sintering and electrical behavior, GDC powders of different composition (3, 6, 8, 10, 12, 15 and 18 mol% GDC) were synthesized by citrate-nitrate gel combustion route. Shrinkage behavior of GDC powders was monitored by a dilatometer. The powders were sintered to get pellets with density above 97% of theoretical density. The dense sintered pellets of different compositions were used for conductivity measurements using a frequency response analyzer. The contributions of bulk and grain boundaries towards the total resistance have been delineated and the conductivity has been explained on the basis of hopping frequency from the complex impedance plot. The activation energies for oxygen ion conduction in the bulk and grain boundary have been determined from the Arrhenius type relationship of conductivity. It was confirmed that maximum ionic conductivity was obtained with 12 mol% GDC. 12GDC pellet sintered at 1200 °C are further heated for grain growth in order to study the effect of grain size on ionic conductivity.

Ultrafine NiO powder for use in anode material was synthesized by solution combustion route. NiO-GDC composition in 50:50 weight ratios was prepared by mixing in a pot mill. Shrinkage behavior of the anode composition was studied using a dilatometer. Electrical conductivity was measured after reduction in hydrogen atmosphere. The effect of sintering temperature on the microstructure and electrical conductivity of Ni-GDC cermet was studied. For estimating the ASR at the interfaces, NiO-GDC electrode and GDC electrolyte have been integrated in symmetric cell form to evaluate the interfacial polarization resistance by ac impedance spectroscopy technique.

Gadolinium cobaltate doped with different percentage of barium was synthesized by solution combustion route as well as solution polymerization method. Based on the process and powder characteristics the later process was chosen for further study. The effect of barium doping on sintering behavior, thermal expansion coefficient and electrical conductivity was studied. Symmetrical cells were prepared and area specific resistance for interfacial polarization was evaluated. The composition and processing parameters were optimized for its application as cathode.

Based on the results of the above studies, anode supported single cells were fabricated by tape casting method. In this electrolyte, anode was integrated by co-casting in tape form and co-firing. Cathode slurry in terpineol medium was painted over the electrolyte followed by sintering. I-V characterization of the single button cell was carried out.



Publications

Publications in Journals out of the present work

1. Combustion synthesis, powder characteristics and shrinkage behavior of ceria gadolinia system, R K Lenka, T Mahata, P K Sinha and B P Sharma, *J. Am. Ceram. Soc.*, 89 (2006)] 3871-3873
2. Combustion synthesis of gadolinia doped ceria using glycine and urea fuels, R K Lenka, T Mahata, A K Tyagi, and P K Sinha *J. of Alloys Comp.* 466(2008) 326-329.
3. Influence of grain size on the bulk and grain boundary ionic conduction behavior in Gadolinia doped Ceria, R.K. Lenka, T. Mahata, A.K. Tyagi and P.K. Sinha, *Solid State Ionics*, 181(2010) 262-267.
4. Synthesis and characterization of GdCoO₃ as a potential SOFC cathode material, R K Lenka, P K Patro, T Mahata, P K Sinha and A K Tyagi, *J. of Alloys and Comp.* 537 (2012) 100-105.
5. Effect of Ba on the performance of GdCoO₃ cathode R.K. Lenka, T. Mahata, A.K. Tyagi and P.K. Sinha, *Solid State Ionics* (communicated).
6. Characterization of Ni-GDC SOFC anode fabricated using nano-powders R.K. Lenka, T. Mahata, A.K. Tyagi and P.K. Sinha, *J. Am. Ceram. Soc.* (communicated).

Conference Presentations

1. Effect of firing temperature on the ionic conductivity in 12 mol% gadolinia doped ceria *presented at PM-08 International Conference and Exhibition held at Chennai on 20 – 21 Feb., 2008.* R.K. Lenka, T. Mahata, P.K. Sinha, and B.P. Sharma 185



Name : **Jayashree Biswal**
Enrolment No. : CHEM01200804004
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : A Study on Synthesis of Silver and Gold Nanoparticles by Employing Gamma Radiation, Their Characterization and Applications

Abstract

Metal nanoparticles (nps) especially noble metal nanoparticles are being explored for application in the areas of sensing, imaging, catalysis and antimicrobial applications. Generation of these metal nps by high energy radiation is promising because of several advantages offered by radiolytic method. It is possible to generate spherical as well as nonspherical nps (nanorods, nanoplates) with controlled size by radiolytic route. Capping agents play very important role in stabilization of metal nps. Both natural polymer and synthetic polymers containing specific functional groups, like -OH, -NH₂, -COOH etc., can stabilize metal nps on their surfaces. The long polymer chain restricts agglomeration of the nps. In this work natural polymer, namely guar gum and synthetic polymer namely, poly methacrylic acid (PMA), poly vinyl pyrrolidone (PVP) have been explored for their stabilization property. Unlike spherical nps, anisotropic nps possess two absorption bands in the electromagnetic spectrum. Small changes in the shape of nanoparticle can have great effect on a variety of physical properties of the material. The key parameter to generate anisotropic nps is dose rate of irradiation along with presence of certain adsorbing molecule like surfactant and some metal ions. These molecules selectively adsorb upon certain facets of growing nanoparticle, blocking those facet and allowing directional growth. The nps were characterized by various techniques, such as uv-visible spectroscopy, XRD, TEM, TG and FTIR. Because of high surface area as well as high surface energy of metal Nps, other molecules easily adsorb upon their surfaces. This property of metal nps helps in Detection and estimation of chemical and biological analytes.

Publications

Journals:

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2. Jayashree Biswal, S.P. Ramnani, R. Tewari, G.K. Dey, S. Sabharwal, (2010) Short aspect ratio gold nanorods prepared using gamma radiation in the presence of Cetyltrimethylammonium bromide (CTAB) as a directing agent, *Radiat. Phys. Chem.* 79, 441–445
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4. Jayashree Biswal, S. P. Ramnani, seema Shirolkar and S. Sabharwal, (2011) Synthesis of rectangular plate like gold nanoparticles by insitu generation of seeds by combining both radiation and chemical methods, *Radiat. Phys. Chem.* 80, 44–49.
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2. Jayashree Biswal, S. Sabharwal, Synthesis and characterization of controlled shape metal nanoparticles by using gamma radiation, International symposium on materials chemistry (ISMC), 7-11 Dec, 2010, BARC, Mumbai, India 121
3. Jayashree Biswal, S. P. Ramnani, S. Sabharwal, Synthesis of Metal Nanoparticles by High Energy Radiation, NAARRI international Conference (NIC), 13-15 Dec, 2010, Mumbai, India.
4. Nilanjali Misra, Jayashree Biswal, S. Sabharwal, Synthesis of Polyvinyl pyrrolidone capped gold nanoparticles by gamma radiolysis, National symposium on radiation and photochemistry (NSRP), 10-12 Mar, 2011, JNV Univ., Jodhpur, India.



Name : **Babita Tiwari**
Enrolment No. : PHYS01200704024
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Thermo-Physical Properties and Structural Aspects of Some Phosphate and Silicate Glasses/Glass-Ceramics

Abstract

Glasses and glass-ceramics are essential materials for many technologically important applications like hermetic sealing and optoelectronic devices etc. This thesis presents studies on glasses and glass-ceramics in the sodium aluminium titano-phosphate (NATP), strontium zinc silicate (SZS) and barium zinc silicate (BZS) systems. The thermo-physical, optical and structural properties have been studied using a combination of DTA, TMA, MH, XRD, FTIR, Raman, MAS-NMR, UV-V is absorption spectroscopy and SEM with EDS. The effect of TiO_2 addition in sodium alumino-phosphate (NAP) glass having potential application in low temperature sealing has been studied. Structure-property correlation indicates that the role of TiO_2 and Al_2O_3 changes from network modifier to network former in NATP glasses around 10 mol% TiO_2 . Surface degradation studies reflect that the partial substitution of P_2O_5 with TiO_2 , results in higher chemical durability of NATP glasses. SZS and BZS glasses and glass-ceramics with different additives have been investigated as potential high temperature sealants for SOFC. Studied compositions of SZS and BZS glasses fulfill the most important criteria (TEC, T_{ds} and η of thermo-physical properties for use as sealants for SOFC. The microstructural evolution with heat treatment revealed the spinodal decomposition for liquid in liquid phase separation in the base SZS glass. Crystallization kinetics study revealed a diffusion controlled bulk crystallization mechanism starts dominating over the bulk crystallization and the activation energy decreases. Lower activation energy indicates a better control over crystallization during sealing process. $\text{Sr}_3\text{Si}_3\text{O}_9$ and $\text{Sr}_2\text{ZnSi}_2\text{O}_7$ crystalline phases formed in all the SZS glass-ceramics and different barium silicate phases formed in BZS glass-ceramics depending on composition. Based upon these studies, compositions with B_2O_3 and V_2O_5 additives have been found most suitable and seals were fabricated with Crofer -22- APU. These seals were found Vacuum compatible at elevated temperatures, even after exposure at 850°C for 800h. In the thesis efforts have been made to show that the thermo-physical properties of the investigated glasses are a sensitive function of structural configurations present in these glasses and can be modified by incorporating suitable additives. Studies also demonstrate the utility of structural/microstructural and thermo-physical characterization in optimization of composition of glasses/glass-ceramics for novel applications like high temperature sealing.

Publications

International Journals: 07 (published) + 2 (accepted) + 3 (to be communicated)

1. Babita Tiwari, and coworkers "Comparison of strontium zinc based and barium zinc based silicate glasses" under preparation.
2. Babita Tiwari, S.C. Gadkari and G.P. Kothiyal, "Studies on crystallization of $\text{SrO-ZnO-B}_2\text{O}_3\text{-SiO}_2$ based glasses", under preparation.



3. Babita Tiwari, M. Pandey, V. Sudarsan, S.C. Gadkari and G.P. Kothiyal, "Thermophysical, crystallization and structural studies of Strontium zinc silicate based glassceramics", to be communicated.
4. Babita Tiwari, S.C. Gadkari and G.P. Kothiyal, "Investigation on Glasses in strontium zinc borosilicate system as sealants for solid oxide fuel cell", *Adv. Mater. Res.* accepted.
5. Babita Tiwari, M. Pandey, S.C. Gadkari and G.P. Kothiyal, "Synthesis and Structural Studies of Multi-Component Strontium Zinc Silicate Glass-Ceramics", *AIP Journal: Confer. Proc.* accepted.
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7. Babita Tiwari, S. Bhattacharya, A. Dixit, S.C. Gadkari and G.P. Kothiyal, "Effect of V_2O_5 on SrO-ZnO- B_2O_3 - SiO_2 Glass-Ceramics for High Temperature Sealant Application", *AIP Journal: Confer. Proc.* 1447 (2012) 575-76.
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9. Babita Tiwari, V. Sudarsan, A. Dixit and G.P. Kothiyal, "Study of Glass/Glass-Ceramics in the SrO-ZnO- SiO_2 System as High Temperature Sealant for SOFC Applications", *Int. J. Hydrogen Energy* 36 (2011) 15002-8.
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12. G. P. Kothiyal, A. Ananthanarayanan, Babita Tiwari, M. Goswami and V. K. Shrikhande, "Studies on some Glasses and Glass-Ceramics for various Applications including Seals", *Mater. Sci. Forum*, 587-588 (2008) 162-166. International/National Conferences: 10
13. Babita Tiwari, A. Sarkar, S. C. Gadkari and G. P. Kothiyal, "Crystallization Kinetics of BaO-ZnO- SiO_2 Glass", 22- AGM of MRSI- Bhopal, Feb-13-16, 2011.
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17. Babita Tiwari, A. Dixit and G.P. Kothiyal, "Study of Glass-Ceramics in the SrO-ZnO-SiO₂ System as High Temperature Sealant for SOFC Applications", International Symposium & Exhibition on Fuel Cell Technologies (FUCETECH 2009), Nehru Centre, Mumbai, Nov. 11- 13, 2009.
18. Babita Tiwari, A Sarkar, and G P Kothiyal, "Thermo-physical properties and crystallization behavior of BaO based silicate glasses for high temperature sealants", National Symposium on Science and Technology of Glass and Glass-ceramics (NSGC-2008), BARC, Mumbai, Oct. 15-17, 2008.
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Name : **Abhinav Saket**
Enrolment No. : PHYS10200604011
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Topological Qubits in Quantum Spin Chains

Abstract

I worked on exactly solvable one-dimensional spin-1/2 chains which are generalised versions of Kitaev's honeycomb model. In the first model, Tetrahedral model, the analytic solutions for the zero Majorana modes has been presented. Localised and unpaired Majorana modes has been shown to occur even in the bulk of the chain. These modes have been created and manipulated tuning Z₂ flux configurations.

The second one dimensional model, I worked on, is XYZ-Ising model. It has been shown that model is analytically solvable for all defect sectors. An alternate proof has been presented that the defect free sector is the ground state, which is valid for a larger parameter range. The defect sectors of the model have degenerate ground states corresponding to unpaired Majorana fermion modes. It has been established that the degeneracy is topologically protected against disorder in the spin-spin couplings.

The unpaired Majorana fermions can be manipulated by tuning the model parameters and can hence be used for topological quantum computation. The physical realisation of the model has been proposed. Using Josephson Junction Quantum Circuits, XYZ-Ising model can be realised.

Publications

1. Abhinav Saket, S.R. Hassan and R. Shankar, Manipulating unpaired Majorana fermions in a quantum spin chain. Phys. Rev. B82, 174409 (2010).
2. Abhinav Saket, S.R. Hassan and R. Shankar. Topological aspects of an exactly solvable spin chain (to be published in PRB).



Name : **Jitendra Bahadur**
Enrolment No. : PHYS01201004005
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Small Angle Scattering Investigations of Nano-Ceramics and Nano-Composites

Abstract

Nano-materials are at the leading edge of the rapidly developing field of nanotechnology. Since last decade, nano-materials in general and nano-ceramics in particular have gained tremendous importance owing to their potential technological applications. It is important to note that the pertinent length scales, which are present in the nano-ceramic and nano-composite systems, manifest in 1-1000 nm range. Small angle scattering is an ideal technique to study the nano-ceramics and self-assembled materials.

In present thesis, two broader aspects of the nanoceramics have been dealt with. First aspect deals with the sintering behavior of the nanoceramics aggregates prepared by sol-gel or precipitation route. Pore morphology in NiO and YCrO₃ nano-ceramic aggregates get modified under sintering. The modification in pore morphology has been attributed to mass transport by atomistic diffusion during sintering. Mesoscopic and microscopic structures under heat treatment has been studied for NiO doped TiO₂ submicrospheres. Sintering behavior of fractal aggregates such as YAG, doped Ceria have been investigated. The experimental results have been understood using Monte Carlo simulation that established that smoothening of fractal rough surface under sintering is possible due to the diffusion transport of materials.

Second aspect of the thesis deals with evaporation induced self-assembly of the nano-particles via spray drying. In recent years, spray drying has been found a special place in synthesizing hierarchically structured grains by atomizing a colloidal suspension into droplets and then converting these droplets into nanostructured grains. The effect of various physico-chemical parameters on the assembly of nanoparticles during drying has been studied. The micrometric grains having various morphologies have been synthesized and characterized.

The spray drying experiments of silica colloids with varying colloidal concentration in slow drying regime showed that overall morphology of assembled grains spherical for all concentration. Further assembly of nanoparticles and their internal arrangement during drying can be modified by addition of electrolyte in initial dispersion. Buckling induced morphological transformation the colloidal droplets to doughnut like grains during EISA of nano-particles under fast drying regime has been shown. Hypothesis based on the formation and buckling of shell of jammed NPs at air-water interface explained the morphological transformation. It has been indicated that reduction in elastic modulus of the formed shell, by incorporation of soft anisotropic colloids, at the air water interface facilitated the buckling. Hollow microcapsules have been synthesized by using EISA of silica colloids and SDS micelles by tuning viscosity of the initial suspension and surface charge on the colloids using hydrotropic aniline hydrochloride. Ordering of surfactant in the assemble microcapsules is demonstrated from SAXS/SANS measurements.



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4. Formation of hollow spherical and doughnut microcapsules by evaporation induced self-Assembly of nanoparticles: Effects of particle size and polydispersity, D. Sen, J. Bahadur, S. Mazumder, S. Bhattacharya, *Soft Matter*, 8, 10036–10044 (2012).
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8. Buckling driven morphological transformation of droplets of a mixed colloidal suspension during evaporation induced self assembly by spray drying D. Sen, J. S. Melo, J. Bahadur, S. Mazumder, S. Bhattacharya, G. Ghosh, D. Dutta and S.F. D' Souza *Eur. Phys. J. E*, 31, 393, 402 (2010).
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10. Evolution of a fractal system with conserved order parameter under thermal annealing J. Bahadur, S. Mazumder, D. Sen, S. Ramanathan, *J. Phys.: Condens. Matter*, 22 195107 (2010).
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12. Effect of Heat Treatment on Pore Structure in Nano-Crystalline NiO: A Small Angle Neutron Scattering Study J. Bahadur, D. Sen, S. Mazumder and S. Ramanathan *Journal of Solid State Chemistry*, 181, 1227–1235 (2008).



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17. *Effects of calcination on microscopic and mesoscopic structures in Ca and Sr doped nanocrystalline Lanthanum Chromites H. Bhatt, J. Bahadur, M. N Deo, S. Ramanathan, K. K Pandey, D. Sen, S. Mazumder, S. M Sharma *Journal of Solid State Chemistry*, 184 204–213 (2011).
18. *Structural characterization of manganese-substituted nano-crystalline zinc oxide using small-angle neutron scattering and high-resolution transmission electron microscopy B. Roy, B. Karmakar, J. Bahadur, S. Mazumder, D. Sen and M. Pal *J. Appl. Cryst.*, 42, 1085–1091 (2009).
19. *Extraction of single scattering profile from multiple small-angle scattering data utilizing basis function set D. Sen, J. Bahadur, S. Mazumder *Eur. Phys. J-B*, 71, 75-84 (2009).
20. *Decoration of carbon nanotubes with metal nanoparticles by wet chemical method: A small-angle neutron scattering study J Bahadur, D Sen, S Mazumder, Jyoti Parkash , D Sathiyamoorthy, R Venugopalan *Journal of Nanoscience and nanotechnology*, 10, 2963–2971 (2010).
21. *Small-Angle Neutron Scattering Investigations on sintering behavior of combustion synthesized La_{0.8}Sr_{0.2}CrO₃, A. K. Patra, J. Bahadur, S. Mazumder, Sathi Nair, R. D. Purohit and A. K. Tyagi, *J. of Nanoscience and Nanotechnology*, 8, 1–6 (2007).
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*Publications not included in the thesis.



Name : **Ranjita Kumari Mohapatra**
Enrolment No. : PHYS07200604027
Constituent Institute : Institute of Physics, Bhubaneswar
Title : Investigating Formation and Evolution of Z(3) Walls and Flow Anisotropies in Relativistic Heavy-Ion Collision

Abstract

Search for the QGP at relativistic heavy-ion collision experiments (RHICE) has reached a very exciting stage with the ongoing experiments at Relativistic Heavy-Ion Collider (RHIC) and the Large Hadron Collider (LHC). One of the important aim of these experiments is to study dynamical details of the quark-hadron phase transition and nontrivial features of QGP. SU(3) pure gauge theory, without dynamical quarks, has Z(3) global symmetry which is restored below T_c in the confined phase and spontaneously broken in the deconfined phase giving rise to three degenerate vacua. Topological defects are inevitably produced in the symmetry breaking phase transitions. These defects are localized regions in which the system is locked in symmetric phase while the whole system is in symmetry broken phase. The formation of different types of topological objects depends upon the vacuum manifold. In confinement-deconfinement phase transition, Z(3) domain walls and the QGP strings (forming at the junctions of three Z(3) walls) are produced. We study the formation of defects via Kibble Mechanism in confinement-deconfinement phase transition in RHICE where Z(3) symmetry is spontaneously broken. These defects can lead to non-trivial consequences in heavy-ion collisions.

The expectation value of Polyakov loop $L(x)$ is an order parameter for confinement deconfinement phase transition. This order parameter transforms non-trivially under Z(3) symmetry and thus gives rise to 3 degenerate vacua in the high temperature phase of SU(3) gauge theory. Using an effective potential based on Polyakov loop order parameter for QCD proposed by Pisarski, we carry out numerical simulations of the evolution of Z(3) walls and strings in RHICE in a first order phase transition. It is known that quark-hadron transition is likely to be a first order transition at large values of baryon chemical potential. Our results are then applicable to such situations, e.g. high baryon density, low energy heavy-ion collisions.

Since strong elliptic flow at RHIC hints towards early thermalisation, the phase transition may not be a equilibrium transition but more likely a quench. During this quench also where the transition proceeds via spinodal decomposition, these defects are produced. We further see bubble like structure in this spinodal decomposition. This is a surprising result because these bubbles are produced even if there is no meta-stable barrier for bubble nucleation between the false vacuum (confined phase) and the true vacuum (deconfined phase). This suggests a new type of phase transition dynamics which needs to be studied in greater detail.

We also have discussed the case where Z(3) symmetry is spontaneously broken leading to degenerate Z(3) vacua. However, real QCD involves dynamical quarks and Z(3) symmetry is explicitly broken due to quarks giving rise to $\theta=0$ being the true vacuum while the other two Z(3) vacua are lifted. $I=0$ vacuum also shifts towards nonzero value along $\theta=0$. When the symmetry breaking is large, the Polyakov loop order parameter field rolls to the true vacuum everywhere in the system. In such a situation we find there are huge oscillations of the field before it settles in the true vacuum. This huge oscillation of the field may affect the elliptic flow. We study this possibility and find that the elliptic flow coefficient v_2 , as well as the spatial eccentricity undergo huge oscillations in this quench scenario compared to the



equilibrium transition situation. These results point out that it is important to take effect of quench induced oscillations of the order parameter field in hydrodynamical simulation to calculate elliptic flow anisotropy.

There are important implications of these defects in relativistic heavy ion collisions. Domain walls and strings melt away when the temperature drops below T_c . However, they may leave their signatures in the distribution of final particles due to large concentration of energy density in extended regions as well as nontrivial scatterings of quarks and antiquarks with these objects. Due to quark/antiquark reflection inside a collapsing wall, each reflection increases the momentum of the enclosed particle. This leads to a specific pattern of P_T enhancement of quarks with heavy flavors. The modification of P_T spectrum of resulting hadrons can be calculated and the enhancement of heavy hadrons at high P_T be analysed for the formation of Z(3) walls. Domain walls are extended along z direction. Hence the correlation of particle production over a large range of rapidity are expected from such extended regions. Z(3) walls and strings may not only provide qualitatively new signatures for the QGP phase, but may prove the first laboratory study of such topological objects in a relativistic quantum field theory system.

Elliptic flow is one of the most important signatures of QGP. Here we show that elliptic flow anisotropy in relativistic heavy-ion collisions can be analyzed using a certain technique of shape analysis of excursion sets recently proposed by us for CMBR fluctuations to investigate anisotropic expansion history of the universe. The technique analyzes shapes (sizes) of patches above (below) certain threshold value for transverse energy/particle number (the excursion sets) as a function of the azimuthal angle and rapidity. Angles with maximum difference in the two distributions identify the event plane, and the magnitude of difference in the two distributions relates to the magnitude of momentum anisotropy, i.e. elliptic flow. This is an important analysis technique which quantifies the elliptic flow anisotropy.

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1. "Super-horizon fluctuations and acoustic oscillations in relativistic heavy ion collisions", A.P. Mishra, R.K. Mohapatra, P.S. Saumia and A.M. Srivastava; Phys. Rev. C 77, 064902 (2008).
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4. "Enhancement of flow anisotropies due to magnetic field in relativistic heavy-ion collisions", R.K. Mohapatra, P.S. Saumia and A.M. Srivastava; Mod. Phys. Lett. A 26, 2477 (2011).
5. * "Analyzing flow anisotropies with excursion sets in heavy-ion collisions", R.K. Mohapatra, P.S. Saumia and A.M. Srivastava; Mod. Phys. Lett. A 27, 1250168 (2012).
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7. “ Effects of quarks on the formation and evolution of Z(3) walls and strings in relativistic heavy-ion collisions”, U.S. Gupta, R.K. Mohapatra, A.M. Srivastava and V.K. Tiwari; Phys.Rev. D 86, 125016 (2012).
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*“Bubble formation during spinodal decomposition in heavy-ion collisions”, S. Digal, R.K. Mohapatra; Pre-print in preparation.

(*) indicates papers on which this thesis is based.

Conference Proceedings

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3. “Simulation of first order confinement transition in relativistic heavyion collision”, U.S. Gupta, R.K. Mohapatra, A.M. Srivastava and V.K. Tiwari; Indian J. Phys. 85, 115-121 (2011).



Name : **Amit Kumar Singh Gautam**
Enrolment No. : LIFE09200604009
Constituent Institute : Tata Memorial Centre, Parel, Mumbai
Title : Biochemical and Biophysical Analysis of Substrate Recognition,
Global Unfolding and Degradation by Eukaryotic Proteasome

Abstract

Almost every cellular pathway involved in the biology of an eukaryotic organism is homeostatically regulated by the Ubiquitin Proteasome System (UPS). Eukaryotic 26S proteasomes are multi-subunit multi-specific ATP dependent protease. In order to dissect the hierarchical steps in proteasomal degradation, identify the sequence and structural requirements as well as the rate limiting steps in proteasomal degradation, we have developed an *in vitro* model system using purified 26S proteasomes and apomyoglobin (apoMb). To the best of our knowledge, this is the first report wherein we successfully demonstrated the inherent ability of purified 26S proteasome to degrade a globular protein (apoMb) *in vitro* in the absence of ubiquitin, adaptor or other trans-acting elements. Heme bound form of Mb was not recognized and degraded by proteasome; removal of heme exposes a previously buried F-helix which is dynamic in nature. This floppy F-helix sensitizes the proteasomal ATPases to the presence of the substrate. ApoMb is then anchored to the proteasome primarily through A-helix; it is further stabilized by additional interactions with B-helix and CD-loop. Degradation is initiated by insertion of the floppy F-helix in the form of a loop into the central channel. Adjacent helices are unraveled by AAA+ ATPases of proteasome to generate an unstructured region long enough to reach the active site chamber. Using peptide panning, competition experiments and structural guided approach we have identified key residues in the A-helix that anchors apoMb to the proteasome. The findings from the study besides confirming the requirement for unstructured regions in degradation offers the following new insights: a) origin and identification of an intrinsic degradation signal in the substrate, b) identification of sequences in the native substrate that are likely to be responsible for direct interactions with the proteasome, and c) identification of critical rate limiting steps like exposure of the intrinsic decon and destabilization of an unfolding intermediate that are presumably catalyzed by the ATPases.

Publications

Publication from thesis

Published

1. Amit Kumar Singh Gautam, Satish Balakrishnan, Prasanna Venkatraman (2012) Direct and Ubiquitin independent recognition and degradation of a folded protein by the eukaryotic proteasomes- origin of intrinsic degradation signals. PLoS ONE 7(4): e34864. Doi:10.1371/journal.pone.0034864.

Other publications

2. Vinita Wadhawan, Yogesh A Kolhe, Nikhil Sangith, Amit Kumar Singh Gautam and Prasanna Venkatraman (2012). Biochemical Journal. From prediction to experimental validation-Desmoglein 2 is a functionally relevant substrate of matriptase in epithelial cells and their reciprocal relationship is important for cell adhesion.



Name : **Subrata Majumder**
Enrolment No. : PHYS07200604024
Constituent Institute : Institute of Physics, Bhubaneswar
Title : Studies of Nanostructures, Ion Beam Patterned Surfaces and their Interaction with DNA

Abstract

The studies presented in this thesis demonstrate the formation TiO₂, ZnO and Hg nanostructures and their interactions with DNA. The oxide (TiO₂, ZnO) and Hg nanostructures display immense potential for numerous applications in the fields of photocatalysis, optical and electronic devices, magnetic recording media and biosensors. The formation of nanostructures, here, has been undertaken by a variety of routes for creating self assembled structures. The modifications in the conformations of DNA molecule, through interaction with these nanostructures, have also been investigated here. studied here. The metal oxide TiO₂ (110) and ZnO , nanostructure, studied here, show several unique properties. The nanostructures created on the TiO₂ surfaces show enhanced optical properties in the visible as well as in the UV regime. The Oxygen vacancies created during the sputtering process have been shown to be primarily responsible for these enhanced photocatalytical properties. These nanodot patterned surfaces also display higher biocompatibility and hydrophilicity. The ZnO nanostructures display room temperature ferromagnetism in the absence of any magnetic doping. The larger nanostructures show very strong long range magnetic ordering at room temperature. The Oxygen vacancies created, during growth, are primarily responsible for these observations. The larger nanostructures are also more biocompatible, with DNA displaying more stable conformations on them. Self assembled Hg nanostructures have been fabricated through the conjugation within the DNA double strands. The interaction between the Hg nanostructures and DNA has been investigated and the results show that Hg exclusively interacts with the nitrogen bases of the DNA and not with the phosphate backbones. Formation of two specific metal-base compounds as well as the modification in the transport properties, after interaction of Hg with DNA, have been demonstrated here. Both these properties display that DNA can be used as a sensor of mercury.

Publications

Published and Communicated in Journals

1. *"Ion irradiation induced nano pattern formation on TiO₂ Single Crystal", S. Majumder, D Paramanik, V Solanki, I Mishra, D.K. Avasthi, D Kanjilal, and Shikha Varma, *Appl.Surf.Sci* 258, 4122-4124 (2012).
2. *"Bandgap Tailoring of Rutile TiO₂ (110) via Surface patterning with ECR sputtering", Subrata Majumder, D. Paramanik, V. Solanki, B.P. Bag, and Shikha Varma, *Appl. Phys. Lett.* 98, 053105 (2011).
3. "Formation of Patterns and Scaling Properties of Tantalum Surfaces after Low Energy
4. Ion Beam Irradiation", Subrata Majumder, R. Medicherla, D. Paramanik, V. Solanki, I. Mishra, and Shikha Varma, *Rad. Eff. Def. Solids.* 166, 592-597 (2011). *"ZnO Nanocrystals: Magnetic Study", S. Majumder, V. Solanki, A. Gupta and Shikha Varma, *Asian jour. of Phys.*, 19, (2 & 3), 269 (2010).
5. *"Fabrication, photoemission studies, and sensor of Hg nanoparticles templated on plasmid DNA", Subrata Majumder, M. Priyadarshini, U. Subudhi, M. Umananda, G. B. N. Chainy, P. V. Satyam, and



- Shikha Varma, *Appl. Phys. Lett.*, 94, 073110 (2009). Also appeared in • *Nature India* 68, February 27, (2009). • *Virtual Journal of Biological Physics Research*, 17, 5, March 1 (2009)
6. * "X-Ray Photoelectron Spectroscopic Investigations of Modifications in Plasmid DNA after Interaction with Hg-Nanoparticles", S. Majumder, M. Priya-darshini, U. Subudhi, G.B.N. Chai and Shikha Varma, *Appl. Surf. Sci.*, 256 438-442(2009).
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 8. "Studies of self-organized Nanostructures on InP(111) surfaces after low energy Ar⁺ ion irradiation", D. Paramanik, S. Majumder, S. R. Sahoo, S. N. Sahu and S. Varma, *Journal Of Nanoscience And Nanotechnology*, 8, 4227-30 (2008).
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 10. "Formation of self organised Ta nano-structures by argon ion sputtering of Ta foil: XPS and AFM study", V.R.R. Medicherla, S.Majumder, D. Paramanik and Shikha Varma, *The Journal of Electron Spectroscopy and Related Phenomena*, 180, 1-5 (2010).
 11. "Vertically aligned Mn-doped Zinc Oxide nanorods by hybrid wet chemical route", R.N. Gayen, S. Majumder, S. Varma, and A. K. Pal, *Mater.Chem. Phys.* 123, 138- 146, (2010).
 12. "Scaling Studies Of Nano Dots Formed On InP(111) Surfaces Via MeV Implantations", D. Paramanik, S. R. Sahoo, S. Majumdar and S. Varma, *Jour. of Nanoscience and Nanotechnology*, 8, 4207 (2008).
 13. "Size Dependant Electronic Structure from InP Nanodots", D. Paramanik, S. R. Sahoo, *Subrata Majumder* and Shikha Varma, *Vacuum*, 1-55(2009).
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 15. "Surface plasmon characteristics of nanocrystalline gold/DLC composite films prepared by plasma CVD technique", R. Paul, S. Hussain, S. Majumder, S. Varma and A. K. Pal, *Mater. Sc.& Engg. B*,164,156-164,(2009).
 16. "Effect of substrate temperature on implantation doping of Co in CdS nanocrystalline thin films", S.Chandramohan, A. Kanjilal, S. N. Sarangi, S. Majumder, R. Sathyamoorthy, C.-H. Hong, and T. Som, *Nanoscale*, 2, 1155-1159 (2010).
 17. "Effect of Fe-ion implantation doping on structural and optical properties of CdS thin films", S.Chandramohan, A. Kanjilal, S. N. Sarangi, S. Majumder, R. Sathyamoorthy, and T. Som, *Appl. Phys. A*, 99, 837-842 (2010).
 18. "Implantation-assisted cobalt doping induced modifications in structural, optical, and vibrational properties of CdS thin films", S. Chandramohan, A. Kanjilal, S.N. Sarangi, *Subrata Majumder*, R. Sathyamoorthy, T. Som, *Journal of Applied Physics*, 106, 063506 (2009).
 19. "Surface roughness and power spectral density study of SHI irradiated ultra-thin gold films", P. Dash, P. Mallick, H. Rath, A. Tripathi, Jai Prakash, D.K. Avasthi, S. Mazumder, S.Varma, P.V. Satyam and N. C. Mishra, *Appl. Surf. Sci.*,256(2009) 558-561.
 20. "Size Scaling Properties of Nanostructures Produced By Ion Sputtering", *Subrata Majumder*, D. Paramanik, and Shikha Varma, *Phys. Rev. Lett.* (2012) (under review).
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Conference Proceedings

1. "Developing Nano-patterns on InP(111) surfaces after keV irradiation", S.Majumder, Dipak Paramanik, S.R.Sahoo, Shikha Varma, *DAE Solid State Physics Symposium*, December 26-31,(2006), Barkatullah University,Bhopal, India
2. "Time evolution of Nano-dots on InP(111) surfaces by 3 keV Ar ion Sputtering", D. Paramanik, S.Majumder, S. R. Sahoo and S. Varma, *Mat. Res.Soc. Symp. Proc.* 1020,GG04 (2007), April 9-13, Material research Society Spring Meeting, San Francisco, USA.
3. "Utilizing Ion Beams For Forming Nanostructures On InP Surfaces, D. Paramanik", S. Majumder, S. R. Sahoo, S. K. Choudhury and Shikha Varma, *Mesoscopic, Nanoscopic, and Macroscopic Materials (IWMNMM)*, *AIP conf. Proc.* 1063(2008)239.
4. "Evolution Of Surface Topography On GaAs(100) And GaAs(111) At Normal And Oblique Incidence Of Ar Ions", V. Venugopal, P. Das, T. Basu, S. Garg, S.Majumder, S. N. Sarangi, S. R. Bhattacharyya, T. K. Chini, and T. Som, *AIP Conf. Proc.*, 1276, 50, (2010) (International Conference on Advanced Nanomaterials and Nanotechnology (ICANN-2009))
5. "Reduction of Anatase TiO₂ on Si(111) by Ion Beam Sputtering", V.R.R. Medicherla, R.R. Mohanta, K.L. Mohanta, Nimai C.Nayak, S. Choudhary, S.Majumder, V. Solanki, Shikha Varma, D.M. Phase, and V. Sathe, *AIP Conf. Proc.*, 1461, 403 (2012).



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Title : Electrochemistry of Boron Deposition from Fluoborate Containing Mixed Chloride-Fluoride Melts

Abstract

An Ag/AgCl reference electrode developed for studying the electrochemistry of fluoroborate containing chloride-fluoride melts was shown to be reversible, stable and non-polarizable over the temperature range 1073 to 1123 K. The reduction potentials of Fe^{2+}/Fe and Ni^{2+}/Ni in the melt KF-KCl were obtained over the temperature range 1073 – 1123 K.

The electrochemical reduction of $\text{B(III)} + 3\text{e} \rightarrow \text{B}$ in KCl (81.54 mol%)-KF (18.45mol%)- KBF_4 (1.6 to 7.73×10^{-4} mol cm^{-3}) and KCl (18.54 mol%)-KF (18.45 mol%)- NaBF_4 (1.67×10^{-4} mol cm^{-3}) melts on a Pt electrode (over the temperature range 1073 to 1123 K) occurred by a single-step three-electron process. Boron electrodeposited on Pt electrode at 1073 K was found to be amorphous in nature.

Linear sweep voltammetric studies were carried out to determine the concentration of oxide ion in KCl-KF melts. The purpose of the study was to determine the effectiveness of this technique for the titration of oxide ions (O^{2-}) in molten chloride-fluoride melts released by sodium oxide additions.

The progress of the electrowinning of boron from the melt KCl – KF – KBF_4 was investigated by assaying the aqueous solutions of the salt residues withdrawn from the melt at periodic intervals. A systematic investigation on the electrowinning of boron was reported. Empirical reactions were formulated in order to arrive at the most probable reaction scheme during the course of the electrolysis. The reaction scheme was possibly influenced by many factors including the melt composition and the source of boron etc.

Publications

International Publications:

1. Electrochemistry of deposition of boron from KCl-KF-KBF₄ melts: Voltammetric studies on platinum electrode, Rahul Pal, S. Anthonysamy, V. Ganesan, *Journal of The Electrochemical Society*, 159, 6, F157 - F165 (2012).
2. Description of the melt stoichiometry in the electrodeposition of boron from KCl-KF-KBF₄ melts, Rahul Pal, K. Ananthasivan, S. Anthonysamy, V. Ganesan, *Electrochimica Acta*, 61, 165 – 172 (2012).
3. Development and electrochemistry of a novel Ag/AgCl reference electrode suitable for mixed chloride-fluoride melts, Rahul Pal, K. Ananthasivan, S. Anthonysamy, V. Ganesan, *Electrochimica Acta*, 56, 4276 – 4280 (2011).
4. Electrochemistry of deposition of boron from KCl-KF-NaBF₄ melt, Rahul Pal, S. Anthonysamy (Communicated)
5. Voltammetric determination of oxide ion in KCl-KF melts, Rahul Pal, S. Anthonysamy (Manuscript under preparation)



List of conference and symposia papers:

International conferences and symposia:

1. An Ag/AgCl reference electrode suitable for electrochemical studies in chloridefluoride melts, Rahul Pal, K. Ananthasivan, S. Anthonysamy, V. Ganesan, ISAEST-9, Chennai, 2-4 December, 2010. 159

National conferences and symposia:

1. Determination of oxide ion impurity in KCl-KF melt by linear sweep voltammetry, Rahul Pal, S. Anthonysamy, NCE16, PSGR College, Coimbatore, 15-16 December 2011.
2. Determination of fluorooxoborate species in boron containing mixed chloridefluoride melts using linear sweep voltammetric (LSV) technique, Rahul Pal, S. Anthonysamy, CRSM, IGCAR, Kalpakkam, 14-15 July, 2011.
3. Electrochemistry of boron deposition from KCl-KF-KBF₄ melt: Voltammetric studies on a platinum electrode, Rahul Pal, K. Ananthasivan, S. Anthonysamy, V. Ganesan, Indo-Italian Workshop on Frontiers of Fundamental and Industrial Electrochemistry: The Challenge of Science for a Better World, University of Delhi, Delhi, 30 - 31 August, 2010.
4. Optimisation of some of the process parameters for the production of elemental boron through electrowinning process, Rahul Pal, K. Ananthasivan, S. Anthonysamy, V. Ganesan, MR09, IIT Mumbai, 2-5 May, 2009.



Name : **Bishnu Prasad Kar**
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Title : Conformations of Molecules Containing π Systems: Matrix Isolation Infrared and *Ab Initio* Studies

Abstract

Conformations arise due to the different spatial orientation of atoms in a molecule, where one form can interconvert to another, through rotation around formally single bonds. In fact, when a single bond is flanked between two double bonds, the rotational barrier is comparatively higher than an isolated single bond, due to conjugation. The rotational barrier is still higher when one non-bonding p-orbital is in conjugation with a double bond, due to ease of delocalization of the p-orbital. Five molecules containing π bond(s) were studied in this work. Stilbene, which involves a π -system and three organic carbonates which involve n- π system, were studied using matrix isolation infrared spectroscopy and *ab initio* methods. The organic carbonates studied were dimethyl carbonate (DMC), diethyl carbonate (DEC) and diphenyl carbonate (DPC). Another n- π system containing molecule Dimethoxy silanone (DMSi), a silicon analogue of dimethyl carbonate was studied for its conformations using *ab initio* computations. These molecules are studied in order to understand the conformational behavior of systems with backbone C-O-(X=O)-O-C, where X= C, Si and P. Phosphorous containing systems (phosphates) have studied earlier in our lab.

These molecules were trapped in inert gas matrixes (Ar, Kr and N₂) at ~10 K on a KBr substrate. An effusive nozzle source heated at different temperatures was used to deposit the mixture of matrix gas and sample vapor. Deposition was also performed using a supersonic jet source. These experiments were performed to alter the population of different conformations in matrix. In order to observe the photoisomerization, in a few systems, UV-Visible light from a broad band source was irradiated on the matrix isolated samples. IR spectra of matrix isolated samples evidenced the presence of different conformations. *Ab initio* computations at B3LYP/6-31++G** level along with Natural Bond Orbital (NBO) analysis and atoms-in-molecules (AIM) calculations were used to study these molecules theoretically.

When matrix isolated cis-stilbene was irradiated with UV-visible light from a broad band source, evidences obtained through IR spectroscopy, showed the presence of both non-planar and planar trans-stilbene in matrix as the photoisomerization products. Conversion of non-planar form of trans-stilbene to the planar form on annealing evidenced that later is more stable than former. Planar and non-planar forms of trans-stilbene were observed due to rotations of phenyl rings. In the study of DMC, the ground state (cis-cis) and first higher energy (cis-trans) conformer were trapped in the low temperature matrixes. The hindered rotations around MeO-C bonds are the reason of different conformations in DMC. In DEC, different orientations of terminal methyl groups and the rotations around EtO-C bonds, together describe the detail conformational landscape. The IR spectra of matrix isolated DEC were assigned to four conformers. A few features were assigned for higher energy conformers which were different from those of ground state conformer. In DPC, both phenyl ring rotation and the rotation around PhO-C bond are the cause of different conformations in molecules. However, only the ground state conformer was identified in matrix. Computation study on conformations of DMSi, showed a similar conformational behavior as in DMC. A comparison study of DMC, DMSi and trimethyl phosphate (TMP) on the basis of NBO analysis, showed a greater participation of d orbital of phosphorous in bonding, which resulted in strong geminal and vicinal delocalization interactions, and in turn, determined the conformational preferences in the phosphate. DMC-H₂O and DEC-H₂O, 1:1 complexes



were also studied here. In both cases, the carbonyl complexes, where H₂O was H-bonded to carbonyl oxygen, were found to be more exothermic than the alkoxy complexes, where H₂O was attached to alkoxy oxygen.

Publications

Journals

1. Matrix Isolation FTIR Studies of Non-Planar Trans-Stilbene, Bishnu Prasad Kar, N. Ramanathan, K. Sundararajan, K. S. Viswanathan, *Journal of Molecular Structure*, 2011, 994, 364-370.
2. Conformations of Dimethyl Carbonate and its Complexes with Water: A Matrix Isolation Infrared and *ab initio* Study, Bishnu Prasad Kar, N. Ramanathan, K. Sundararajan, K. S. Viswanathan, *Journal of Molecular Structure*, 2012, 1024, 84-93.
3. Conformations of Diethyl Carbonate: A Matrix Isolation Infrared and *ab initio* Study, Bishnu Prasad Kar, N. Ramanathan, K. Sundararajan, K. S. Viswanathan. (manuscript in preparation).
4. Conformations of Diphenyl Carbonate: A Matrix Isolation Infrared and *ab initio* Study. (manuscript in preparation).

Conference presentations

1. Non-planar trans-stilbene trapped in inert gas solids, Bishnu Prasad Kar, K. S. Viswanathan, Poster presentation, Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters, Goa, India, February 18-21, 2010.
2. Conformations of dimethyl carbonate and its complexes with water: A matrix isolation and *ab initio* study, Bishnu Prasad Kar, K. Sundararajan, N. Ramanathan, K. S. Viswanathan, Poster presentation, Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters, Uttarakhand, India, February 18-20, 2011.
3. Conformations of dimethyl carbonate: A Matrix isolation infrared and *ab initio* study, Bishnu Prasad Kar, N. Ramanathan, K. Sundararajan, K. S. Viswanathan, Oral presentation, Chemistry Research Scholar's Meet, Indira Gandhi Centre for Atomic Research, Kalpakkam, India, July 14-15, 2011.
4. Conformations of diethyl carbonate: A Matrix isolation infrared and *ab initio* study, Bishnu Prasad Kar, N. Ramanathan, K. Sundararajan, K. S. Viswanathan, Poster presentation, International Conference on Vistas in Chemistry, Indira Gandhi Centre for Atomic Research, Kalpakkam, India, October 11-13, 2011.
5. Conformations of diphenyl carbonate: A Matrix isolation infrared and *ab initio* study, Bishnu Prasad Kar, N. Ramanathan, K. Sundararajan, K. S. Viswanathan, Poster presentation, Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters, Bengaluru, India, February 17-19, 2012.



Name : **Trinadha Raja Pilladi**
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Title : Studies on the Synthesis and Characterization of Nanocrystalline Boron Carbide

Abstract

Commercially boron carbide is synthesized by carbothermic reduction of boric oxide/boric acid. However, this method is energy inefficient and requires very high temperatures. The product obtained is in the form of nuggets and coarse-grained. Hence, this product is subsequently crushed and intensively milled to produce powder. The milled powder is inherently associated with contamination resulting from the grinding media and hence requires an acid leaching for purification. In addition, this process results in substantial loss of boron in the form of its oxides due to volatilization at high temperatures. Hence, the resultant final product, boron carbide, is often found to contain a significant amount of residual carbon. It is a challenge to synthesize boron carbide without free carbon residue for various industrial applications. Thermodynamic equilibrium calculations on carbothermic reduction of boric oxide were carried out using FactStage 6.2. The stability boundaries pertaining to B_2O_3 (1), $B_4C(s)$, $B_4C(1)$, B(s), B(1) and C(s) have been evaluated as a function of temperature and C to B_2O_3 mole ratio. The results of these calculations identified the most favourable conditions of temperature and C to B_2O_3 mole ratio for the synthesis of carbon-free boron carbide through carbothermic reduction of boric oxide. A low-temperature synthesis of boron carbide by carbothermal synthesis is possible by improving the dispersion of boric oxide and carbon components. Carbothermal reduction of boric oxide uniformly distributed in carbon matrix obtained through the pyrolysis of suitable gel precursors is an attractive low-temperature method for the synthesis of boron carbide. Studies were carried out to synthesize nanocrystalline boron carbide from various gel precursors.

The lattice thermal expansion of nanocrystalline and microcrystalline boron carbides has been measured by high temperature X-ray diffraction technique in the temperature range 298-1773 K. The lattice parameters of both were found to increase with increase in temperature. A new method was developed for the digestion of boron carbide for its chemical assay. The new digestion technique developed in this study facilitates relatively fast and accurate determination of total boron, its isotopic content and trace elements present in it.

Publications

1. Synthesis of nano crystalline boron carbide from boric acid–sucrose gel precursor Trinadha Raja Pilladi, K. Ananthasivan, S. Anthonysamy and V. Ganesan Journal of material science, 47 (2012) 1710-1718
2. Thermal expansion of nanocrystalline boron carbide Trinadha Raja Pilladi, G. Panneerselvam, S. Anthonysamy and V. Ganesan Ceramic international, 38(2012) 3723-3728
3. Development of a digestion method for the analysis of boron carbide Trinadha Raja Pilladi, R. K. Prabhu and S. Anthonysamy Communicated to Current Analytical Chemistry.
4. Thermodynamic analysis of carbothermic reduction of boric oxide Trinadha Raja Pilladi, K. Ananthasivan and S. Anthonysamy Manuscript under preparation.



5. Synthesis of boron carbide from boric oxide – sucrose gel precursor, Trinadha Raja Pilladi, K. Ananthasivan and S. Anthonysamy Communicated to Powder Technology.

Conferences:

1. Synthesis of boron carbide Trinadha Raja Pilladi, K. Ananthasivan, S. Anthonysamy and V. Ganesan Proceeding of National symposium for Material research scholars (MR09), IIT Bombay, 2009
2. Synthesis of nano crystalline boron carbide from boric acid–sucrose gel precursor Trinadha Raja Pilladi, K. Ananthasivan, S. Anthonysamy and V. Ganesan, Proceeding of International Conference on Nanomaterials and Nanotechnology (NANO-2010), Tiruchengode, 2010
3. Synthesis of nano crystalline boron carbide from boric acid–sucrose gel precursor Trinadha Raja Pilladi, K. Ananthasivan, S. Anthonysamy and V. Ganesan Chemistry Research Scholars Symposium (CRSM), Kalpakkam, 2011.
4. Thermodynamic analysis of carbothermic reduction of boric oxide Trinadha Raja Pilladi, K. Ananthasivan, S. Anthonysamy and V. Ganesan, International Conference in Vistas in Chemistry(ICVC), Kalpakkam, 2011
5. Participated in National symposium on Chemistry for Societal and Environmental Needs, Central Leather Research Industry, Chennai, August 29-31, 2011



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Title : Studies on Dynamics of Space Charge Dominated Beam in a Low Energy Beam Transport System

Abstract

In this thesis, detailed analytical and numerical studies have been performed to study the dynamics of space charge dominated beams (single species and multispecies) propagating through the low energy beam transport line.

In the first part of the thesis a self consistent kinetic description has been used to understand the dynamics of a space charge dominated beam in an aligned and misaligned solenoid based transport system. A general equation for the centroid motion is derived using the nonlinear Vlasov-Maxwell equation. It has been shown that there exists a self-consistent Vlasov equilibrium distribution in the case of a uniform beam density. The beam envelope equation with respect to centroid is similar in form to the K-V envelope equation when the conducting beam pipe is considered very far away from the beam.

The microwave proton sources produce a proton along with major unwanted components are H_2^+ and H_3^+ . The presence of these unwanted species in an intense beam alters the dynamics of the primary species during the transport. A multispecies beam envelope model of an axisymmetric space charge dominated multispecies beam has been developed for the evolution of the radius of each species along the transport line. The effects of the slit are taken into account in the beam envelope model. The envelope model can be utilized for a precise estimate of the beam envelope, without using particle in cell methods.

An optimization method based on the random search method has been developed to find the optimal beam line settings for the transport and matching of the desired primary beam and rejection of unwanted species at the slit using the developed multispecies beam envelope model.

A detailed analysis has been carried out for the longitudinal and transverse beam dynamics of intense beams during the beam bunching. The longitudinal dynamics and transverse dynamics have been studied using disc model and envelop model respectively for various types of fixed shape density profiles. The beam envelope equation has been modified for short bunches comparable to beam radius to take into account the longitudinal space charge effect.

A 2D PIC code has been developed for self-consistent beam dynamics study of space charge dominated beam (single and multispecies) in beam transport line. The PIC code has been used to investigate the dynamics of beam with different types of distributions in aligned and misaligned solenoid based transport system. The PIC code has also used to get detailed information about the evolution of the beam distribution and emittance growth in the case of multispecies beams. It has been shown that the rejection of unwanted species is very effective when the slit is placed after the hollow formation of the unwanted species. A 3D PIC code has also been developed to study the dynamics during the longitudinal compression.



Publications

1. * "Simulation of beam bunching in the presence of space charge effects", P. Sing Babu, A. Goswami, and V. S. Pandit, Nucl. Instrum. Methods Phys. Res. A 603, 222 (2009).
2. * "Optimization of sector geometry of a compact cyclotron by random search and matrix methods", P. Sing Babu, A. Goswami, P. R. Sarma, and V. S. Pandit, Nucl. Instrum. Methods Phys. Res. A 624, 560 (2010).
3. * "Behavior of space charge dominated beam during longitudinal compression in a bunching system", P. Sing Babu, A. Goswami, and V. S. Pandit, Nucl. Instrum. Methods Phys. Res. A 642, 1 (2011).
4. * "Envelope equations for cylindrically symmetric space charge dominated multispecies beam", P. Sing Babu, A. Goswami, and V. S. Pandit, Phys. Plasmas 18, 103117 (2011).
5. * "Effect of nonuniform radial density distribution on space charge dominated beam bunching", P. Sing Babu, A. Goswami, and V. S. Pandit, Phys. Plasmas 18, 113104 (2011).
6. * "A Vlasov Equilibrium for Space Charge Dominated Beam in a Misaligned Solenoidal Channel", P. Sing Babu, A. Goswami, and V. S. Pandit, Phys. Plasmas 19, 080702 (2012).
7. * "Optimisation of beam line parameters for space charge dominated multi species beam using random search method", P. Sing Babu, A. Goswami, and V. S. Pandit, Phys. Lett. A 376, 3192 (2012).
8. * "Studies of space charge dominated multispecies beam in a solenoid based beam transport line", P. Sing Babu, A. Goswami, and V. S. Pandit, Phys. Plasmas 19, 113112 (2012).
9. * "Self consistent study of space charge dominated beam in a misaligned transport system", P. Sing Babu, A. Goswami, and V. S. Pandit, Submitted to journal.
10. * "Effect of subdominant species on the evolution of intense primary beam in a low energy beam transport line", P. Sing Babu, A. Goswami, and V. S. Pandit, Submitted to journal.
11. "Estimation of the transverse space charge limiting current in a compact isochronous cyclotron", V. S. Pandit, and P. Sing Babu, Nucl. Instrum. Methods Phys. Res. A 523, 19 (2004).
12. "Behavior of space charge dominated beam in a high current compact cyclotron", A. Goswami, P. Sing Babu, and V. S. Pandit, Nucl. Instrum. Methods Phys. Res. A 562, 34 (2006).
13. "Transfer matrix of a Glaser magnet to study the dynamics of nonaxisymmetric beam", A. Goswami, P. Sing Babu, and V. S. Pandit, Nucl. Instrum. Methods Phys. Res. A 678, 14 (2012).
14. "Investigation on beam envelope oscillations and amplitude growth in a high current compact cyclotron", A. Goswami, P. Sing Babu, and V. S. Pandit, Eur. Phys. J. Plus 127: 47 (2012).
15. "Beam focusing characteristic of an elliptical solenoid magnet in the presence of space charge", A. Goswami, P. Sing Babu, and V. S. Pandit, Nucl. Instrum. Methods Phys. Res. A 685, 46 (2012).
16. "Space charge dominated beam dynamics in a spiral inflector for a compact cyclotron", A. Goswami, P. Sing Babu, and V. S. Pandit, Eur. Phys. J. Plus 127: 79 (2012).
17. "Self-consistent space charge dominated beam dynamics in a spiral inflector", A. Goswami, P. Sing Babu, and V. S. Pandit, Nucl. Instrum. Methods Phys. Res. A 693, 276 (2012).
18. "Transport characteristics of a glaser magnet for an axisymmetric and non-axisymmetric space charge dominated beam", A. Goswami, P. Sing Babu, and V. S. Pandit, Phys. Plasmas 19, 123105 (2012).



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Title : Primordial Features and Non-Gaussianities

Abstract

Currently, inflation is the most promising paradigm to describe the origin of the perturbations in the early universe. Most models of inflation permit a sufficiently long epoch of slow roll inflation, which, in turn, leads to a featureless, nearly scale invariant, power law, primordial scalar spectrum. Such a spectrum, along with the assumption of a spatially flat, concordant Λ CDM [i.e. involving the cosmological constant Λ and Cold Dark Matter CDM]] background cosmological model, provides a good fit to the recent observations of the anisotropies in the Cosmic Microwave Background (CMB) by missions such as the Wilkinson Microwave Anisotropy Probe (WMAP).

Even though, as a broad paradigm, inflation can be termed as a success, it would be fair to say that we are still some distance away from converging upon a specific model or even a class of models. There exist a wide variety of inflationary models that remain consistent with the data.

While a nearly scale invariant, power law, scalar spectrum fits the observations of the anisotropies in the CMB quite well, there exist a few data points at the lower multipoles, which lie outside the cosmic variance associated with the conventional power law primordial spectrum. Statistically, a few outliers in a thousand or so data points are always expected. However, these outliers can be handy from the phenomenological perspective of attempting to constrain the models from the data, since only a more restricted class of inflationary models can be expected to provide an improved fit to these outliers. Therefore, it is a worthwhile exercise to explore models that lead to certain deviations from the standard power law, inflationary perturbation spectrum, and also provide a better fit to the data.

Over the last few years, it has been recognized that primordial non-Gaussianity can act as a powerful probe to help us discriminate further between the various inflationary models. For instance, it is known that slow roll inflation driven by the canonical scalar fields leads only to a small amount of non-Gaussianity. But, recent analyses of the WMAP data seem to suggest that primordial non-Gaussianity may possibly be large. Ongoing missions such as Planck are expected to determine the extent of non-Gaussianity in the CMB more accurately. It is known that models which lead to features also generate a reasonably large amount of non-Gaussianity. One of the aims of this thesis work has been to systematically explore inflationary models that give rise to specific features in the perturbation spectrum which result in an improved fit to the data, and also lead to observed (or, observable) levels of non-Gaussianity.

Broadly, this thesis can be divided into two parts. While the first part can be said to be devoted to the signatures of features and non-Gaussianities on the CMB, the second focuses on their possible observational imprints in the matter dominated epoch. In the first part, we shall begin with a discussion on the generation of localized as well as non-local features (i.e. characteristic and repeated patterns that extend over a wide range of scales) in the inflationary scalar power spectrum that lead to a better fit to the CMB data than the more standard power law spectrum. We shall also investigate the bi-spectra that result in such scenarios, and study as to how they compare with the current observational limits on the non-Gaussianity parameter f_{NL} . In this context, we shall also discuss the effects of preheating in single



field inflationary models on the evolution of the bi-spectrum. In the second part of the thesis, after considering the effects of primordial features on the formation of halos, we shall discuss the possibility of utilizing the observations of the Ly- α forest towards constraining primordial non-Gaussianity.

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Title : Study of Intermediate Mass Fragment Emission in Heavy-Ion Reaction

Abstract

Lots of studies have been done to search the origin of intermediate mass fragment (IMF) in heavy-ion as well as light-ion reactions. But emission mechanism of IMF are not well understood, particularly in light heavy ion reaction (typically, $A_{\text{projectile}} + A_{\text{target}} \leq 60$) at moderate bombarding energy ($E_{\text{lab}} < 10$ MeV/A). This might be due to strong overlap between elemental yields of different processes in light heavy ion systems. Situation becomes more complicated for α -cluster system, where nuclear structure is known to play an important role in the emission of IMF. In these cases, in addition to the standard fusion-fission route of fragment emission, the projectile and the target have a finite probability to form a long-lived dinuclear composite, which directly undergoes scission (without the formation of the fully equilibrated compound nucleus) to emit complex fragments. This process, termed as nuclear orbiting. The main aim of the present thesis was to study of the effects of the nuclear structure of the colliding light-heavy ions in the emission of IMF which is one of the most active fields in low-energy nuclear physics. Two experiments have been performed for this purpose. An experimental facility has also been developed to continue this study at intermediate energy range.

IMFs Li, Be, B emission have been studied in α -clustered system ^{16}O (117, 125, 145, and 160 MeV) + ^{12}C . The yields of the fragments Li and Be have been found to be in agreement with statistical-model predictions. However, the measured yield of B has been found to be enhanced compared to the theoretical prediction of the same. The enhanced yield of fragment B near entrance channel, indicates the survival of orbiting-like process in $^{16}\text{O} + ^{12}\text{C}$ system at these energies. As orbiting is related to large deformation, quadrupole deformation parameter of the composite system has also been extracted from measured α particle evaporation spectra for the same reactions using light charged particle spectroscopy. Large deformation has been obtained in each case, which may be another possible indication of survival of dinuclear orbiting.

The IMFs Li, Be, B emitted from α -clustered system ^{12}C (77 MeV) + ^{28}Si , non α -clustered systems ^{11}B (64 MeV) + ^{28}Si , and ^{12}C (73 MeV) + ^{27}Al (all having same excitation energy of ~ 67 MeV), have also studied. The aim was to explore and compare the effect of clustering in the fragment emission process in both type of systems, α and non- α clustered. The fully energy damped (fusion-fission) and partially energy damped (deep inelastic) components of the fragment energy spectra have been extracted. It has been found that the yields of fully energy damped fragments ($3 \leq Z \leq 5$) are in conformity with the respective statistical model predictions. Even the yields of FF fragments emitted from α -cluster system, $^{12}\text{C} + ^{28}\text{Si}$, also match with extended Hauser-Feshbach model (EHFM) predictions. The time scales of various deep inelastic fragment emissions extracted from the angular distribution data for the above reactions and have been found to be similar. The angular momentum dissipation in deep inelastic collision has been estimated from the data and it was found to be close to the corresponding sticking limit value.



Several large experimental facilities are being built as a part of the K500 Superconducting Cyclotron(SCC) utilization program at VECC which will enable to continue IMF studies in the Fermi Energy domain. I have, as a part of my thesis work, contributed to the design, development, installation, testing of the large multipurpose reaction chamber which will cater to the needs of different types of experiments using these experimental facilities as well as other detector systems. It is a large (1m diameter, 2.2m long), Segmented, Horizontal Axis, Reaction Chamber (SHARC) which can be pumped down to a nominal pressure of $\sim 5 \times 10^{-7}$ mbar in ~ 8 hours by means of two turbo-molecular (1000 1/s) and two cryo pumps (2500 1/s) backed by two mechanical pumps (37m³/hr). The vacuum

System and movement of target ladder both can be controlled by PLC (Programmable Logic Controller) in auto and manual modes with dynamic display of complete status. Special technique has been developed to fabricate flange with multiple flat ribbon connectors as a feed-through for detectors placed within SHARC. The installation and testing of SHARC has been completed and presently it is connected and aligned with the beam line of SSC.

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Title : Probing Quark Gluon Plasma Through Photon, Dilepton and Strangeness Productions in Relativistic Nuclear Collisions

Abstract

This thesis is addressed with the results of simulation works carried out to settle some of the physics issues related with the injection and acceleration of space charge dominated beam in a compact cyclotron. The design issues of a spiral inflector, main magnet and space charge effect on the behavior of beam envelope in the inflector and cyclotron, where the beam from the ion source has energy of 80 keV and current in the range of 10-20mA.

To optimize the pole profile of the hill of the cyclotron magnet an iterative technique is developed. Here the sector shape is approximated by a polynomial function of radius and minimized the frequency error by optimizing the coefficients of the polynomial by using random search technique. Compared to the other method, it is found that this method gives smooth pole shape of the hill and takes less computation time for optimization and requires only 5-8 parameters for restricting the relative frequency error to 1 in 10^4 .

The design of a spiral inflector in a non-homogeneous magnetic field has been carried out which will be used to deflect 80 keV, 5 mA protons to the median plane of the 10 MeV cyclotron. The central ion trajectories of the spiral inflector are analyzed by using a computer code developed by us. From the results of the central ion trajectories the parameters of the inflector are adjusted in order to orient the beam properly at the exit of it.

A numerical simulation technique has been developed for studying the behavior of beam envelope during the first turn and also to estimate the vertical acceptance of the cyclotron central region in the presence of linear space charge. The change in the beam envelope has been studied by changing the injected beam current, initial width and divergence and emittance of the beam. A proper matching condition has been found and the limit on the injected beam current has also been estimated. The result of simulation indicates that one must have large injection energy ($\sim 80\text{keV}$) and dee voltage ($\sim 100\text{KV}$) to transport 10 mA beam current.

A detailed investigation on the amplitude growth and oscillations in the beam envelopes along the accelerated central particle orbit in the cyclotron has been carried out by using coupled beam envelope equations with acceleration and assuming the beam as a uniform ellipsoidal bunch. The study has been done by changing the current of the injected beam, as well as the initial width and divergence of the beam. The proper matching conditions of the beam have been optimized to reduce the emittance growth at the exit of the inflector. Simulation results show that a converging non-axisymmetric beam with equal emittances at the entrance is desirable to reduce the emittance growth at the exit.

Finally, since the overall goal of this work is to maximize the amount of beam that could be injected into the cyclotron, a transverse beam matching at the inflector entrance was considered to have better beam transmission through it. It is shown that the elliptical solenoid magnet can be used for this purpose. In this work the beam optical properties of an elliptical solenoid magnet has been performed and then feasibility of using an elliptical solenoid for transverse matching of a space charge dominated beam to the acceptance of a spiral inflector has been discussed.



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1. Behavior of space charge dominated beam in a high current compact cyclotron; A. Goswami, P. Sing Babu and V. S. Pandit, Nuclear Instruments and Methods in Physics Research A 562 (2006) 34.
2. Simulation of beam bunching in the presence of space charge effects; P. Sing Babu, A. Goswami and V. S. Pandit, Nuclear Instruments and Methods in Physics Research A 603 (2009) 222.
3. *Optimization of sector geometry of a compact cyclotron by random search and matrix method; P. Sing Babu, A. Goswami, P. R. Sarma and V. S. Pandit, Nuclear Instruments and Methods in Physics Research A 624 (2010) 560.
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* Indicates publications related to this thesis.



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Title : Electronic Structure Studies of Graphite Systems and Some Transition Metal Oxides

Abstract

In this thesis, we have studied the occupied and unoccupied electronic structures of single crystal graphite and highly oriented pyrolytic graphite (HOPG) using angle resolved photoelectron spectroscopy (ARPES) and K-resolved inverse photoemission spectroscopy (KRIPES) respectively. The experimental bands have been compared with theoretical band structures computed by us using tight binding method. The electronic structures of single layer grapheme and bilayer grapheme have also been investigated using tight binding calculations to build up a formalism to be used for the band calculation of graphite. In these calculations emphasis was given on various in-phase coupling and minimum no of inter-phase coupling.

Using ARPES, we find two clearly dispersing bands (\square and \blacklozenge) along the symmetry directions Γ -K and Γ -M of the graphite brillouin zone. The agreement of our results is good near the zone boundaries (the K and M points) with the calculated band structure for which interactions of electrons up to third nearest neighbors (in--plane) are considered and near the zone centre (the Γ point) the agreement is better with the calculated bands having first nearest neighbor interaction only. We estimated a splitting of ~ 0.5 eV between the two valence \square bands of single crystal graphite from its near Fermi energy spectra at the K point. This splitting is due to the weak interlayer coupling in graphite. A sharp peak below E_F at the K point at low temperature comes up which is due to coupling of electrons with photon, indicating a strong electron-phonon coupling. In HOPG the valence band dispersions were taken along different radial directions of its Brillouin zone and we found no azimuthal dependence of the spectra due to its inherent azimuthal disorder. The conduction band structures for both the systems obtained by using KRIPES superimpose well on the theoretical conduction band structure of graphite along Γ -M direction.

Further, the occupied electronic structures of Pb doped multiferroic material, ($\text{Bi}_{1-x}\text{Pb}_x\text{FeO}_3$) and Sr doped $\text{Sm}_{0.1}\text{Ca}_{0.9}\text{MnO}_3$ (a colossal magnet or resistive material) have been studied using UPS, XPS and ResPES techniques.

The valence band electronic structure of the $\text{Bi}_{1-x}\text{Pb}_x\text{FeO}_3$ ($x= 0.02$ to 0.15) system have been studied by using X-ray and ultra-violet photoelectron spectroscopy. As this system undergoes a R3c to cubic phase transition with Pb doping, the near Fermi level states show an enhanced oxygen 2p character due to the weakening of the Fe 3d - O 2p - Bi 6p hybridization strength. The valence bands of compositions with the R3c structure were found to be qualitatively similar to the LSDA calculations except for their estimates of the band width and band gap. One reason for this could be the higher value of effective Coulomb interaction.

Finally, we have studied the electronic structure of $\text{Sm}_{0.1}\text{Ca}_{0.9}\text{MnO}_3$ ($x=0.0, 0.2, 0.3, 0.4$ and 0.6) system, an electron-doped CMR material using ultra violet photoelectron spectroscopy (UPS) and resonance photoelectron spectroscopy (ResPES) with varying photon energy across the Mn 2p-3d absorption edge. The magnetic ground state of the parent compound ($\text{Sm}_{0.1}\text{Ca}_{0.9}\text{MnO}_3$) at low temperatures consists of ferromagnetic clusters (FM) embedded in a G-type AFM phase. But this FM components is very



sensitive to the substitution of Sr for Ca. From the combined UPS and ResPES studies we find that the valence band of this material has major contribution from Mn 3d states and a strong hybridization is there between Mn 3d t_{2g} and O 2p states. With strontium doping, the A site cation size increases and a significant change in the Mn 3d spectral weight is observed which indicates that there is a change in Mn 3d – O 2p hybridization strength due to structural modification caused by Sr doping.

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2. *Towards Phonon Spectrum of Graphene*, Rupali Kundu, arXiv:0710.2077v2 (2007).
3. *Pseudogap behavior of phase-separated Sm_{1-x}Ca_xMnO₃: A comparative photoemission study with double exchange*, P. Pal, M. K. Dalai, R. Kundu, B. R. Sekhar and C. Martin; Phys. Rev. B 77, 184405 (2008)
4. *Electronic structure of Pr_{1-x}Ca_xMnO₃ system revealed by photoemission and inverse photoemission spectroscopies*, M. K. Dalai, P. Pal, R. Kundu, B. R. Sekhar, S. Banik, A. K. Shukla, S. R. Barman, C. Martin, Physica B, 405, (2010), 186-191
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6. * *Tight-binding parameters for graphene*, Rupali Kundu; Mod. Phys. Lett. B 25, (2011) 163-173, DOI: 10.1142/S0217984911025663.]
7. * *Electronic structure of Bi_{1-x}Pb_xFeO₃ from photoelectron spectroscopic studies*, R. Kundu, P. Mishra, B. R. Sekhar, J. Chaigneau, R. Haumont, R. Suryanarayanan and J. M. Kiat; Solid State Communications 151, (2011) 256-258.
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(*) indicates papers on which this thesis is based.



Name : **Jajati Kesari Nayak**
Enrolment No. : PHYS04200704008
Constituent Institute : Institute of Physics, Bhubaneswar
Title : Electronic Structure Studies of Graphite Systems and Some Transition Metal Oxides

Abstract

According to the Big Bang model of cosmology the entire micro-second old universe was in a state of quark gluon plasma (QGP). Even in the present day the quark gluon plasma state is believed to exist in the core of the compact stellar objects like neutron star. Such a novel state of matter is expected to be created in the laboratory by colliding two heavy nuclei at relativistic energies. The possibility of formation of QGP in such collisions have been studied in this thesis using electromagnetic radiations such as real photons & virtual photons (or lepton pairs) and using strange hadrons like K mesons & Λ baryons. The yield of photons, lepton pairs (e^+e^- or $\mu^+\mu^-$) and strange hadrons have been evaluated theoretically and compared with the available experimental data to know about the nature of the matter produced at different colliding energies. The photon productions in terms of transverse momentum (pT) spectra have been evaluated for Pb+Pb collisions at center of mass energy, $\sqrt{s_{NN}} = 17.3$ GeV at Super Proton Synchrotron (SPS), CERN, and for Au+Au collisions at $\sqrt{s_{NN}} = 200$ GeV at Relativistic Heavy Ion Collider (RHIC) energy have been compared with the experimental data measured by PHENIX collaboration. The pT spectra of lepton pairs have also been evaluated for all the energies mentioned above. The evaluations for the pT and invariant mass (M) spectra of $\mu^+\mu^-$ pair productions from In+In collisions at SPS energy have been compared with the data obtained by NA60 collaboration. While evaluating the photon and lepton pair production, the space time evolution of matter has been considered using ideal relativistic hydrodynamics. It is found that the theoretical evaluations with an initial QGP phase explains the experimental observations made by NA60 and PHENIX collaborations at SPS and RHIC energies respectively. We have also evaluated the ratio of the pT spectra of photons to lepton pairs to get rid of some of the uncertainties involved in the initial conditions of the collisions. It has been shown that the ratio of both spectra with proper choice of pT and M window give better information of the initial temperature of the system formed in the collision. This thesis also focuses on the extraction of radial flow (v_r) of the medium using both photon and dilepton spectra. It has been noticed that v_r increase with M up to mass $\sim M_p$ and then decreases gradually (for mass window $M < 1.2$ Ge Low Mass Region) indicating the presence of two types of thermal sources in the matter produced in heavy ion collision. This has been studied for $\sqrt{s_{NN}} = 17.3$ GeV, 200 GeV and 7 TeV respectively for SPS, RHIC AND LHC energies. The strangeness productions have also been considered to probe the matter created in this relativistic nuclear collisions. The ratio of strangeness to the total entropy arguably differentiates the matter produced with and without QGP. Here the yield of strange hadrons like K^+ , K^- and Λ have been computed using Boltzmann transport equation. The theoretical results for K^+/π^+ , K^-/π^- , Λ/π have been compared with the data measured by CERES, NA49 and STAR collaborations for AGS (Alternating Gradient Synchrotron), SPS and RHIC energies. The results show a non-monotonic behavior of the ratio K^+/π^+ , Λ/π with colliding energies when an initial partonic phase is assumed beyond certain threshold in energy, while a monotonic rise is seen for hadronic initial conditions for all energies.



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8. Kaon and Lambda productions in relativistic heavy ion collisions, Jajati K. Nayak, S. Banik and J. Alam, Nucl. Phys. A, 862-863, 286 (2011), Preprint : Nucl-th/1101.3187.
9. Muon pairs from In+In collision at energies available at the CERN Super Proton Synchrotron, Jajati K. Nayak, J. Alam, T. Hirano, S. Sarkar and B. Sinha, Phys. Rev. C, 85, 064906 (2012). Preprint : Nucl-th/0902.0446.

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4. Probing quark gluon plasma through the radial flow of the thermal electromagnetic radiations, Jajati K. Nayak, Payal Mohanty, Jan-e Alam & Santosh Das, Proceedings of ICPAQGP-2010 .
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Name : **Swapnalee Baruah Thakuria**
Enrolment No. : ENGG01200704034
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Title : Investigations on Subcritical and Supercritical Natural Circulation Phenomena Relevant to Advanced Reactors

Abstract

Many new generation reactors incorporate passive or inherent safety systems that utilize natural circulation which require no active controls or operator intervention. The heat transport capability of natural circulation loops is directly proportional to the flow rate it can generate. The reported generalized flow equation applicable for single-phase natural circulation is only valid for cases when the natural circulation loop is either fully laminar or fully turbulent. It is possible that a natural circulation loop can be partly laminar and partly in transition or turbulent flow. In such cases, a single friction law is not applicable throughout the loop. In the present study, a generalized flow equation is proposed for cases where a single friction law is not applicable for the entire loop. The proposed equation is tested with experimental data generated in a uniform diameter rectangular loop. Subsequently the equation is tested with data reported in the literature.

Stability analysis reported in literature for single-phase loops are either for laminar or turbulent flows. In practice, in natural circulation loops, all the flow regimes like laminar, transition and turbulent are observed. Therefore, it is required to develop a stability map, which is valid for all the three regions. In the present work, such a stability map is presented.

Another concept of advanced reactor design is the use of fluids at supercritical pressure condition in both forced and natural circulation systems. For thermodynamically supercritical loops, explicit correlation for steady state natural circulation flow is not available. While using the subcritical natural circulation flow equation for supercritical data, it was not able to predict the steady state flow accurately near pseudo critical region. A generalized correlation has been proposed to estimate the steady state supercritical CO₂ and water data. Subsequently the equation is tested with data reported in the literature for different working fluids.

Sharp change of fluid properties such as density in the critical region gives rise to instability concerns. Consequently, there is considerable interest to investigate the conditions leading to instability. In the present work, analysis has been carried out to predict the threshold of excursive instability and obtained the stability map.

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6. Swapnalee B.T., P.K.Vijayan, 2010, Simulation of single-phase natural circulation instability in a rectangular loop using CFD code PHOENICS, Poster presentation on 20th National and 9th International ISHMT-ASME Heat and Mass Transfer Conference, Mumbai, India.



Name : **Narender Singh Rawat**
Enrolment No. : PHYS01200704029
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Title : Characterization of TL/OSL Phosphors and Study of Photo-Ionization Cross-Sections of Meta-Stable Trap Levels- An Experimental and Theoretical Approach

Abstract

Due to mounting societal anxiety associated with nuclear radiation based energy security the monitoring of the radiation workers has become a serious concern. Thermoluminescence (TL) and Optically Stimulated Luminescence (OSL) based luminescence dosimetry has emerged as the most viable solution to this owing to its inherent operational simplicity and cost effectiveness. Need of a simple and comprehensive approach capable of simultaneous evaluation of all the TL parameters has inspired and led to the theoretical formulation of a novel method which is based on Initial Rise and can be used to analyze general order TL glow peak. This method standalone is capable of yielding all the parameters of a TL glow peak viz. s , E , s' and b . Its experimental validation on CaSO_4 : Dy constitute important ingredient of this research work.

Photo-ionization cross-section being the key parameter to judge the dosimetric performance of an OSL phosphor, its dependence on dose and temperature has been extensively investigated in Al_2O_3 :C. Vacuum assisted post growth thermal impurification (PGTI) technique is an avenue to defect engineer alumina and study the correlation of the defect structures and their concentrations with dosimetric performance. OA and PL studies have shown the requisite abundance of F and F^+ centers. Photo-ionization cross-section (PI-CS) increases with dose and the observed trends of dose dependence of PI-CS could be successfully explained by model involving three OSL traps and their competition. PI-CS increases with Temperature (follows Arrhenius nature) and readout at elevated temperature (TA-OSL) can offer improvement in dose detection limits. Thermal assisted energy for dosimetry OSL traps is evaluated to be 0.03eV. Another approach in the form of non linear light modulation (NL-OSL) has been identified that offers reduction in noise levels. NL-OSL also allows multiple dose readout and a better resolution of OSL peaks in Al_2O_3 :C. Al_2O_3 :C in combination with ^6LiF and HDPE as neutron converters has been demonstrated to be a viable option for neutron dosimetry. Through TL, OSL, PL and EPR correlation studies on MgAl_2O_4 : Tb^{3+} , Tb^{3+} has been identified as luminescent center, F^+ as recombination center and defects responsible for TL peaks to be hole traps. Ag as a co-dopant acts as a sensitizer and Cu as an activator in LBO:Cu, Ag. Our studies and their conclusions have added LBO:Cu, Ag to the list of legitimate OSL phosphors.

Publications

Papers in international/refereed Journals (included in thesis)

1. N. S. Rawat, M. S. Kulkarni, D. R. Mishra, B. C. Bhatt, C. M. Sunta, S. K. Gupta, D.N. Sharma. Use of Initial Rise Method to analyze a General Order Kinetic Thermoluminescence Glow Curve. *Nuclear Instruments and Methods in Physics Research B* 267 (2009) 3475–3479
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8. M.S. Kulkarni , N.S. Rawat , S.V. Thakare , K.C. Jagadeesan, D.R. Mishra, K.P. Muthe, B.C. Bhatt, S.K. Gupta , D.N. Sharma. TL and OSL studies on neutron irradiated pure $\alpha\text{-Al}_2\text{O}_3$ single crystals. *Radiation Measurements* 46 (2011) 1704-1707
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2. N. S. Rawat, M S Kulkarni, D R Mishra, K P Muthe and S K Gupta. Dose dependence studies of photo-ionisation cross-section for $\alpha\text{-Al}_2\text{O}_3\text{:C}$ single crystals. *Proceedings of National Conference on Luminescence and its Applications (NCLA-2010)*
3. N.S.Rawat, D.R.Mishra, G.D.Patra, S.C.Gadkari, S.K.Gupta, M.S.Kulkarni. Elevated temperature Optically stimulated Luminescence Studies on Cu and Ag doped $\text{Li}_2\text{B}_4\text{O}_7$ Single Crystals. *IARPNC 2012 held at Mangalore University*

Papers in international/refereed Journals (not included in thesis)

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Name : **Krishnan Rajkumar**
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Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Zeros of General L-Functions on the Critical Line

Abstract

We study the gaps between consecutive zeros on the critical line for the Riemann zeta function $\zeta(\sigma)$ and certain generalizations of $\zeta(\sigma)$, namely, the Epstein zeta function and the Selberg class of functions. We first give a simplified exposition of a result of Iwaniec and Jutila on the large gaps between consecutive zeros of $\zeta(\sigma)$ on the critical line. We then present a generalization of this result to the case of the Epstein zeta function $\zeta_Q(s)$ associated to a certain binary, positive definite, integral quadratic form $Q(x,y)$. We next establish the analogue of Hardy's theorem, namely that there are infinitely many zeros on the critical line, for degree 2 elements of the Selberg class of L -functions whose Dirichlet coefficients satisfy certain mild growth conditions. We conclude with a conditional version of Hardy's theorem for the degree d elements of the Selberg class for the case $d > 2$.

Publications

1. with Anirban Mukhopadhyay and Kotyada Srinivas) On the zeros of functions in the Selberg class, *Funct. Approx. Comment. Math.* 38 (2008), part 2, 121{ 130.
2. with Anirban Mukhopadhyay and Kotyada Srinivas) On the zeros of the Epstein zeta function. *Proceedings in honour of Prof. T. C. Vasudevan, RMS Lecture Note Series, No. 15 (2011), pp. 73{87.*
3. with Debashish Bose, C.P. Anil Kumar and Shobha Madan) On Fuglede's conjecture for three intervals, *Online J. Anal. Comb.* No. 5 (2010), 24 pp.
4. with Kotyada Srinivas) Zeros of functions in the Selberg class with degree $d > 2$. Preprint.



Name : **MeghmalnarAvinash Manekar**
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Constituent Institute : Raja Ramanna Centre for Advanced Technology, Indore
Title : On Phases of DNA, Entanglement, and Persistence

Abstract

The work presented in this thesis is based on the study of physical properties of Fe-Rh and related pseudobinary alloys, which show interesting functionalities like the giant magnetocaloric effect, giant magnetostriction and giant magnetoresistance governed by a temperature and magnetic field induced first order magneto-structural transition (FOMST) near room temperature. It was reported earlier that though the Fe-Rh alloy shows such wide range of important functional properties, some functionalities like the giant magneto-caloric effect vanish after the first field cycle. In this work we solve this long-standing problem and show that the possible role of phase coexistence and associated metastability across the FOMST in tuning the functional properties of this material has largely gone unnoticed. The phase coexistence and metastability across the first order transition in the parent Fe-Rh alloy were imaged at sub-micron length scales to highlight the fact that these features are generic to any first order transition. Such phase coexistence and metastability across the FOMST in Fe-Rh alloys give rise to interesting thermomagnetic history effects. We also argue that these thermomagnetic history effects which arise across a disorder influenced first order transition are actually common to any other first order transition induced by both temperature and magnetic field and are not limited to only the Fe-Rh system. The understanding of these history effects was used to obtain a large refrigerant capacity of nearly 492.8 J kg^{-1} at room temperature in a Ni doped Fe-Rh alloy, which is probably the largest in any material at this temperature. The other generalization that is attempted is to find the similarity between the nucleation and growth dynamics across a first order transition with the crystallization process of solids. This knowledge is further used for modeling the minor hysteresis loops generated under multiple temperature cycling across the first order transition in one of the Ni doped Fe-Rh alloys. Different kind of thermomagnetic history effects were observed across the temperature driven transition when the amount of disorder is increased in form of higher concentration of Ni doping. The kinetics of the first order ferromagnetic to antiferromagnetic phase transition appear to be arrested in such cases. It was found that the product phase itself might influence its further growth thereby leading to the arrest of the kinetics of the first order phase transition, which is similar to a glass-like state.

Our thesis highlights that, apart from having a large value of the functional property, it is necessary to understand the nucleation and growth mechanism across a first order phase transition, if such materials are to be used for reproducible technological applications under multiple temperature or magnetic field cycles.

Publications

In Refereed Journals:

1. Imaging of time evolution of the first-order magneto-structural transition in Fe-Rh alloy using magnetic force microscopy M. Manekar, C. Mukherjee and S. B. Roy
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2. Thermomagnetic history effects across the first order magneto-structural transition in the giant magnetocaloric Fe-Rh alloy M. Manekar and S. B. Roy Eur. Phys. J. B, vol. 64, p. 19 (2008).
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7. Thermo-magnetic history effects in the giant magnetostriction across the first order transition and minor hysteresis loops modeling in $\text{Fe}_{0.955}\text{Ni}_{0.045}\text{Rh}$ alloy M. Manekar V. K. Sharma and S. B. Roy J. Phys.: Condens. Matter, vol. 24, p. 216004 (2012).

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1. Phase coexistence and its implications on the functional properties of the room temperature giant magnetocaloric alloy Fe-Rh M. Manekar Proceedings of the 53rd DAE Solid state physics symposium, (BARC, Mumbai) p. 25 (2008) (Invited talk).



Name : **Poulomi Sadhukhan**
Enrolment No. : PHYS07200604029
Constituent Institute : Institute of Physics, Bhubaneswar
Title : Magneto - Structural Transition and Magnetic Field Induced in Fe-Rh Based Pseudobinary Alloys

Abstract

In this thesis we study non-equilibrium stochastic paths, especially in the context of the unbinding transition of polymers and DNA. The phases and the phase transitions of DNA being the main attraction, we study the same under a force for both equilibrium and non-equilibrium cases. In course, we study an even simpler two-state system, the Ising ferromagnet, to obtain similar results. The results of a DNA system often show similarities to other systems. For example, the phase diagram resembles that of superconductors, an imaginary time transformation makes the polymer problem equivalent to a quantum problem. Such connections to other topics, which are apparently or mechanism-wise different, are explored.

In the first chapter, we show that a thermodynamic study can produce the features of the zipping-unzipping phase diagram of a dsDNA. We look at the interface between the zipped and the unzipped phases and classify the existing DNAs into two types in terms of the sign of the interface energy. Our study shows that considering the helical order along with the external force under certain circumstances can even make the unzipping transition second order. This fact along with the phase diagram of a DNA matches with that of superconductors. This tempts us to name the two classes as Type I and Type II.

In the second chapter, we study a DNA hairpin and the analogous two-state Ising magnet under a periodic drive. These two systems show similar behavior though the detailed dynamics are different. We find that the simply averaged hysteresis loops suppresses the actual picture of the states. A dynamical phase diagram is proposed which shows the possibility of going from one phase to the other just by varying frequency alone, keeping the amplitude of the external drive fixed.

In the third chapter, we concentrate on the hysteresis of the Ising ferromagnet. Here the aim is to extract the equilibrium discontinuous phase transition curve, which, in a real situation, is difficult to get. To do so, we utilize the work theorem and the histogram method. We show that the work theorem can be obtained from the histogram transformation. Then we generalize the work theorem to an arbitrary number of intensive parameters including the temperature, and express the equilibrium distribution as the principal eigenvector of a specially constructed matrix consisting of the non-equilibrium measurements of the work done. Using this weighted averaging, one can get a much better phase transition curve which cannot be obtained using a simple averaging.

In the fourth chapter, we look at the quantum unbinding transition of a pair of bound quantum particles equivalent to the polymer unbinding transition. For both the short-range and long-range potentials, we compute the von Neumann entropy near the QPT, which diverges negatively. We discuss the behavior of the entropy and its connection to the reunion exponents.

Viewed as a stochastic path, a polymer can be interpreted as a classical random walker with length of the polymer as time. A study of the paths of such a random walker is the topic of the fifth chapter. The classical walker is associated with a power law distribution of the hopping rates. We show that the



quenched and the annealed averaging with the site and the bond disorders give different persistence behaviors, though all have the same behavior for the mean squared displacement.

To summarize, this thesis gives new insights about polymers and DNA problems as these are looked from new angles and the vastness and the universal nature of the polymer problems are brought out.

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4. Dynamical phase transition of a periodically driven DNA; Garima Mishra, Poulomi Sadhukhan, Somendra M Bhattacharjee, Sanjay Kumar. *Phys. Rev. E* **87**, 022718 (2013) . (arXiv:1204.2913)
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7. Persistence of a Brownian walker in disordered media with power law distribution of hopping rates; Poulomi Sadhukhan and Goutam Tripathy (Under preparation).



Name : **Bhramar Chatterjee**
Enrolment No. : PHYS05200704004
Constituent Institute : Saha Institute of Nuclear Physics, Kolkata
Title : Some Local Calculations of Temperatures of Black Hole Horizons

Abstract

A classical black hole absorbs everything but they are capable of thermal radiation coming out of the horizon, which is a quantum process first discovered by Hawking. Almost all the derivations of Hawking radiation depend on the entire spacetime geometry of a black hole. But a black hole horizon can be defined locally, where the laws of black hole mechanics are also applicable. So some derivation of Hawking effect using only the local geometry was in order.

The first attempt in this direction was the tunneling method of calculating Hawking temperature associated with a black hole horizon. In this formalism one calculates the probability of classically forbidden process of s-wave emission across a black hole horizon which has the form of a Boltzmann distribution and thus gives the Hawking temperature. In this work we have shown that as it describes an essentially across the horizon phenomenon, a good set of coordinates is required for the calculations which is regular at the horizon. Though singular coordinates can be used in that case the choice of boundary conditions is crucial in obtaining the correct temperature. We have also found that as long as the metric remains stationary no higher order corrections to the Hawking temperature can be obtained in this method.

The tunneling method has one drawback which is the use of WKB approximation and because of this we have proposed a more general derivation of Hawking effect which is free of such kind of assumptions and depends on the behavior of the field modes near the horizon. Our idea is to construct single particle states only outside the horizon using the field equations and continue them inside the horizon. While crossing the horizon the outgoing modes acquire a logarithmic singularity which can be avoided by considering the distributional properties of the modes. Then the conditional probability that a particle emits when incident on the other side of the horizon gives the expected Hawking temperature associated with the horizon. This method works for the conventional black hole horizons and as well as for the external space times in each case producing the corresponding temperature. We have also applied this method to a fully dynamical space time and found the temperature of this dynamical horizon.

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1. "Tunnelling from black holes in the Hamilton Jacobi approach" Bhramar Chatterjee, Amit Ghosh, P. Mitra (Saha Inst.) Phys. Lett. B 661 (2008) 307-311 [arXiv:0704.1746 [hep-th]]
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5. "Hawking radiation from dynamical horizons" Ayan Chatterjee, Bhramar Chatterjee, Amit Ghosh Phys. Rev. D 87 (2013) 084051 [arXiv:1204.1530 [gr-qc]]



Name : **Rajini P. Antony**
Enrolment No. : CHEM02200704011
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Synthesis, Characterization and Selected Applications of Quasi One Dimensional Nano-Architectures of TiO₂

Abstract

One dimensional nano-architected arrays of TiO₂ has proven to be a promising candidate material because of low cost, non-toxicity, high stability and wide range of applications in the field of energy conversion/storage, electronics, self-cleaning surfaces and environmental photocatalysis. These high aspect ratio arrays constitute a unique class of high performance materials that possess large surface area, directional electron transport, thin tube edges and surface roughness laden with trapped air columns. Vertically aligned nano-tubular titania array with all the above properties is an efficient candidate material for several high technology areas like dye sensitized solar cells (DSSC), large area electron field emitters, wetting – de-wetting coatings and nano-catalytic support. The last one is very effective in addressing green-energy hydrogen generation by splitting of water and photocatalytic decomposition of organic pollutants in water. Suspensions of large specific surface particles like nanotubes are a preferred configuration for efficient light harvesting capability. The research work undertaken for this Thesis addresses fabrication of such arrays, their characterization and demonstration of above application potentials.

The first part of this Thesis deals with the synthesis of vertically aligned pristine and N-doped TiO₂ nanotube array (TNTA) in the form of thin films. N-doped ones were derived using urea as a nitrogen precursor. The Morphology, crystallinity, composition and band gap of the pristine and N-doped TNTA were investigated by Field Emission Scanning Electron Microscopy (FESEM), X-ray Diffraction (XRD), Transmission Electron Microscopy (TEM), X-ray Photoelectron Spectroscopy (XPS), micro Raman, Photoluminescence and UV-Vis absorption spectroscopy studies. N-doped TNTA were found to be visible light active due to reduction in band gap. Further, studies pertaining to their application as DSSC, large area electron field emitters and hydrophobic ↔ hydrophilic switching surfaces are discussed. The DSSC fabricated using TNTA on foils exhibited higher efficiency than DSSC fabricated using TNTA on conducting glasses. An enhancement in field emission current was found on N-doping due to the presence of interband N-2p states. The physico-chemical processes involved in the photo-induced near super-hydrophobic to super-hydrophilic transition of pristine and N-doped TNTA reveals a combination of mechanisms like surface hydroxyl group reconstruction and surface adsorbed organic destruction. The second part of the Thesis deals with the synthesis of pristine, Pt loaded and C & N - co-doped TiO₂ nanotube powders, their characterization and their application in photocatalytic hydrogen generation by splitting of water and photocatalytic decomposition of organic pollutants in water.

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1. Rajini P. Antony, Tom Mathews, Arup Dasgupta, S. Dash, A. K. Tyagi, and Baldev Raj, "Rapid breakdown anodization technique for the synthesis of high aspect ratio and high surface area anatase TiO₂ nanotube powders," *Journal of Solid State Chemistry* 184 (3), 624-632 (2011).
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 - Rajini P Antony, Tom Mathews, Jobha C Johnson, S. Dash and A. K. Tyagi, "Visible light photocatalytic degradation of Rhodamine 6 G by pure and C and N co- doped TiO₂ nanotubepowders", (*Energy and Environment Focus- Just accepted*)
 - Rajini P Antony, Tom Mathews, S. Dash and A. K. Tyagi, "Kinetics and Physico-Chemical Process of Photo-Induced Hydrophobic \leftrightarrow Super-Hydrophilic Switching of Pristine and N-doped TiO₂ Nanotube Arrays" (*Journal of physical chemistry C, J. Phys. Chem. C*, **2013**, 117 (13), pp 6851–6860)
 - Rajini P Antony, Tom Mathews, S. Dash and A. K. Tyagi, " Effect of tube diameter on the photo-induced antibacterial properties of TiO₂ nanotube arrays" (Communicated- RSc advances)
 - Rajini P Antony, Tom Mathews, S. Dash and A. K. Tyagi, "Photovoltaic characteristics of Dye sensitized solar cells fabricated using TiO₂ nanotube arrays." (Communicated - Solar Energy Materials & Solar Cells)

Conference Presentations

- Rajini P Antony, Tom Mathews, C Ramesh, N Murukesan, S Dash, A K Tyagi, Photo-assisted Hydrogen generation from ethanol-water mixtures by Platinum loaded Titania nanotube catalyst, Third International Conference on Frontiers in Nanoscience and Technology (Cochin Nano 2011, August 14-17, Cochin, India). (Oral presentation)
- Rajini P Antony, Tom Mathews, Sitaram Dash and A K Tyagi. "Effect of annealing temperature on structural and morphological stability of TiO₂ nanotube arrays." ICONSET-2011, 28th-30th Nov, 2011, Satyabhama University, Chennai. (Oral presentation- Best presentation award), IEEE Xplore, Proc. of ICONSET-2011, pp. 326-330, DOI:10.1109/ICONSET.2011.6167974.
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Name : **Sapna V. Iyer**
Enrolment No. : LIFE09200604003
Constituent Institute : Tata Memorial Centre, Parel, Mumbai
Title : Role of Cytokeratins 8 and 18 in Differentiation and Transformation of Epithelial Cells

Abstract

Keratins (K) are cytoplasmic intermediate filament proteins of epithelial cells and changes in their expression pattern have been seen during malignant transformation. Expression of the K8/18 pair is normally seen in the luminal cells of the breast epithelium, and its role in progression of breast cancer is not well understood. There are differing reports about the role of K8/18 pair in breast cancer progression. Thus it was important to study the role of this keratin pair in breast cancer derived cell lines with varying transformation potential. In this study, we have modulated K8 expression in three different breast epithelium derived cell lines: non-transformed MCF10A, transformed but poorly invasive MDA MB 468 and highly invasive MDA MB 435. The up-regulation of K8 in the invasive MDA MB 435 cell line resulted in a significant decrease in proliferation, motility, *in-vitro* invasion, tumor volume and lung metastasis. The down-regulation of K8 in MDA MB 468 resulted in a significant increase in transformation potential, motility and invasion *in-vitro*, while MCF10A did not show any changes in cell transformation assays. The preliminary IHC studies on breast tumor samples suggested that the percentage of K8/18 negative tumors were more in case of recurrent tumors as compared to the non-recurrent ones. The microarray analysis in K8 up/down-regulated clones demonstrated differential expression of specific genes which might be involved in transformation related changes. These results indicate the role of K8/18 in modulating invasion in breast cancer - its presence correlating with less invasive phenotype and absence correlating with highly invasive, dedifferentiated phenotype. Previous work from our laboratory has shown that the keratin pair of K8/18 plays a role in promoting tumor progression in an oral SCC derived cell line. These findings suggest the possibility that the same keratin pair may have dissimilar role in neoplastic progression of cancers derived from different epithelia. Thus the data from the present study may have important implications for prognostication of breast cancer. This information could prove useful in developing therapeutic targets for treatment of breast carcinomas in future.

Publications

1. Accepted: Iyer SV, Dange PP, Alam H, Sawant SS, Ingle AD, et al. (2013) Understanding the Role of Keratins 8 and 18 in Neoplastic Potential of Breast Cancer Derived Cell Lines. PLoS ONE 8(1): e53532. doi:10.1371/journal.pone.0053532.



Name : **Kaushik Banerjee**
Enrolment No. : PHYS04200804001
Constituent Institute : Variable Energy Cyclotron Centre, Kolkata
Title : Study of Nuclear Dynamics using Neutrons

Abstract

The present thesis is an attempt to address some of the important aspects of nuclear structure and reaction dynamics at low energy nuclear reaction using neutron as a probe. In low energy nuclear physics, one of the dominant reaction mechanisms is the formation of compound nucleus and its decay. The decay of compound nucleus can be broadly categorized as fission and evaporation. Both these processes have been studied under the present thesis work. In the first experiment we studied fission dynamics in $^{16}\text{O} + ^{238}\text{U}$ at near barrier energies, with the motivation to study different experimental probes and their sensitivity to identify non-equilibrium fission process from compound nuclear fission. Fission fragment mass distribution and neutron multiplicity have been measured in the experiment. The mass distribution data shows a sudden change in the width of the mass distribution at near barrier energies, which is clear indication of presence of quasi fission. The presence of quasi fission was also reported earlier from the angular measurement data. However neutron multiplicity data were found to be consistent with the statistical model prediction, which indicates absence of quasi fission. The same is also observed in the evaporation residue data measured earlier. It is argued that the first two probes (mass distribution and angular distribution) are more sensitive for highly asymmetric system, whereas all probes would be useful and complimentary to each other for the study of quasi-fission in more asymmetric systems, where quasi-fission is more dominant.

In the second experiment another decay process of compound nucleus i.e. particle evaporation was explored to study nuclear level density and its dependence on angular momentum. In this experiment we have populated ^{119}Sb at excitation energies 31.3 MeV and 42.9 MeV using $^4\text{He} + ^{115}\text{In}$. We measured the evaporated neutrons in coincidence with γ -rays from ^{119}Sb . The measurement of evaporated neutrons in coincidence with the γ -rays multiplicity and its subsequent statistical model analysis revealed interesting features of the spin dependence of nuclear level density. The inverse level density parameter k appears to be decreasing with increase in angular momentum, which indicates a relative increase in nuclear level density with angular momentum. Different aspects of nuclear level density, such as the collective enhancement of NLD and the nuclear shape variation at higher angular momentum have been thoroughly considered to explain the observed trend.

The above experiments were performed with the indigenously developed neutron detectors. As a part of this thesis work, we have developed two types of neutron detectors for neutron energy and multiplicity measurements. Energy measurement is done by time of flight technique using small volume (~ 1.5 litres) liquid scintillator detector, whereas multiplicity measurement is done using Gd loaded large volume (~ 500 litres) liquid scintillator detector.



Publications

(A) Relevant to the present Thesis

In refereed journals

1. "Variation of nuclear level density with angular momentum", K. Banerjee, S.Bhattacharya, C. Bhattacharya, M. Gohil, S. Kundu, T. K. Rana, G. Mukherjee, R. Pandey, P. Roy, H. Pai, A. Dey, T. K. Ghosh, J. K. Meena, S. Mukhopadhyay, D. Pandit, S. Pal, and S. R. Banerjee Phys. Rev. C 85, 064310 (2012).
2. "Evidence of quasi fission in $16\text{O} + 238\text{U}$ reaction at sub barrier energies", K. Banerjee, T.K. Ghosh, S. Bhattacharya, C. Bhattacharya, S. Kundu, T. K. Rana, G. Mukherjee, J. K. Meena, J. Sadhukhan, S. Pal, P. Bhattacharya, K. S. Golda, P. Sugathan, R. P. Singh Phys. Rev. C 83, 024605 (2011).
3. "Variation of neutron detection characteristics with dimension of BC501A neutron detector", K. Banerjee, T. K. Ghosh, S. Kundu, T. K. Rana, C. Bhattacharya, J. K. Meena, G. Mukherjee, P.Mali, D. Gupta, S. Mukhopadhyay, D. Pandit, S. R. Banerjee, S.Bhattacharya, T. Bandyopadhyay, S.Chatterjee, Nucl. Instr. And Meth. A, 608, 440 (2009).
4. "Characteristics of Gd-loaded liquid scintillators BC521 and BC525", K. Banerjee, S. Kundu, S. Mukhopadhyay, T.K. Rana, S. Bhattacharya, C. Bhattacharya, S. R. Banerjee, T.K. Ghosh, G. Mukherjee, T. Bandyopadhyay, A. Dey, J. K. Meena, P. Mukhopadhyay, D. Gupta, S. Pal, D. Pandit, S. Bhattacharya, Nucl. Instr. and Meth. A, 580, 1383 (2007). 139

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2. "Angular momentum gated neutron evaporation studies"**K. Banerjee** et. al., Proc. of DAE -BRNS Symp. on Nucl. Phys., 55, 324 (2010).
3. "Development of liquid scintillator based Neutron Detector", **K. Banerjee** et.al, Proc. of DAE -BRNS Symp. on Nucl. Phys., 51, 624 (2006).
4. "Capture time distribution study in Gd loaded liquid scintillator", **K. Banerjee** et.al, Proc. of DAE -BRNS Symp. on Nucl. Phys., Vol. 51, 588 (2006).
5. "Simulation result of 4π neutron multiplicity detector", **K.Banerjee**, et.al, Proc. of DAE -BRNS Symp. on Nucl. Phys., 50, 440 (2005).
6. "Simulation study of liquid scintillator based 4π neutron detector", **K.Banerjee**, et.al, Proc. of DAE -BRNS Symp. on Nucl. Phys., 49, 524(2004).

(B) Other Publications (in refereed journals)

1. "Measurement and simulation of neutron response function of organic liquid scintillator detector", M. Gohil, K.Banerjee, S. Bhattacharya, C. Bhattacharya, S. Kundu, T. K. Rana, G. Mukherjee, J. K. Meena, R. Pandey, H. Pai, T. K. Ghosh, A. Dey, S. Mukhopadhyay, D. Pandit, S. Pal, S. R. Banerjee, T. Bandopadhyay, Nucl. Instr. and Meth. A 664, 304 (2012).
2. "Complex-fragment emission in low-energy light-ion reactions", S. Kundu, C. Bhattacharya, K. Banerjee, T. K. Rana, S. Bhattacharya, A. Dey, T. K. Ghosh, G. Mukherjee, J. K. Meena, P. Mali,



- S. Mukhopadhyay, D. Pandit, H. Pai, S. R. Banerjee, and D. Gupta Phys. Rev. C 85, 064607 (2012). 140
3. "Measurement of Giant Dipole Resonance width at low temperature: A new experimental perspective", S. Mukhopadhyay, Deepak Pandit, Surajit Pal, Srijit Bhattacharya, A. De, S. Bhattacharya, C. Bhattacharya, K. Banerjee, S. Kundu, T. K. Rana, G. Mukherjee, R. Pandey, M. Gohil, H. Pai, J. K. Meena and S. R. Banerjee, Phys. Lett. B 709, 9 (2012).
 4. "Onset of deformation at $N = 112$ in Bi nuclei", H. Pai, G. Mukherjee, R. Raut, S. K. Basu, A. Goswami, S. Chanda, T. Bhattacharjee, S. Bhattacharyya, C. Bhattacharya, Bhattacharya, S. R. Banerjee, S. Kundu, K. Banerjee, A. Dey, T. K. Rana, J. K. Meena, D. Gupta, S. Mukhopadhyay, Srijit Bhattacharya, Sudeb Bhattacharya, S. Ganguly, R. Kshetri, and M. K. Pradhan, Phys. Rev. C 85, 064317 (2012).
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Name : **Shailesh Lal**
Enrolment No. : PHYS08200604019
Constituent Institute : Harish Chandra Research Institute, Allahabad
Title : Higher-Spin Theories and the AdS/CFT Correspondence

Abstract

The AdS/CFT Correspondence is a remarkable output of string theory---a theory of quantum gravity---which conjectures that a string theory defined on spacetimes that asymptote to Anti de-Sitter (AdS) spaces are actually completely equivalent to a conformal field theory (CFT) which is defined on the spatial boundary of the AdS. Since a conformal field theory is a usual relativistic Quantum Field Theory, which we understand well, this gives us a tool to explore string theory and Quantum Gravity.

This thesis describes our work on the holography of higher-spin theories in AdS. The motivations are two-fold: firstly, in the low-dimensional examples of AdS(3) and AdS(4) these theories are expected to have CFT duals in their own right. These dualities are non-supersymmetric and therefore offer a rare concrete opportunity to explore AdS/CFT in non-supersymmetric settings. Secondly, these arise in the context of a novel and relatively unexplored corner in the landscape of the duality, that of free planar gauge theories, which correspond to tensionless string theory on AdS spacetimes. This is a natural starting point to get insight about the mechanics of AdS/CFT and gauge-string duality. One also expects that in the tensionless limit, there is a sector of the string theory which consists of an infinite tower of massless, interacting particles, which should be described by a consistent classical theory. It is natural to expect that this theory is a Vasiliev theory. Our work in higher-spin theories is with these questions in mind.

An important tool in our exploration of higher-spin theories will be the one-loop partition function of the AdS higher-spin theory, which contains the leading quantum corrections to its classical description. We will define this partition function in terms of the heat kernel of the Laplacian acting on symmetric, transverse traceless tensors of arbitrary rank. A useful tool to exploit is the fact that AdS is a symmetric space, and these questions have a group theoretic interpretation. We use this fact to determine a closed-form expression for the heat kernel of the Laplacian for arbitrary spin fields over quotients of (Euclidean) AdS.

Also, motivated by the Gaberdiel-Gopakumar conjecture relating higher-spin theories in AdS(3) to minimal model CFTs, we consider a topologically massive deformation of these theories. In particular, we compute the one-loop partition function of a topologically massive spin-3 field. This provides us with evidence that the W symmetry survives the chiral limit, which was a question unclear from previous analyses. We expect that these expressions will be an important ingredient in formulating an explicit duality for topologically massive higher-spin theories.

We finally turn to the computation of the partition function of higher-spin theories in AdS(5). We find simplifications in the multiparticle partition function of the non-minimal Vasiliev theory. In particular, for thermal AdS(5), we write the answer in a form strongly suggestive of a vacuum character, and also in a form reminiscent of a higher-dimensional MacMahon function, generalising the observations of Gaberdiel, Gopakumar and Saha for AdS(3). We also turn on chemical potentials for the other AdS(5) Cartans and compute the one-loop partition function. We again obtain a vacuum character-like form for the answer. We take this as evidence that the asymptotic symmetry algebra of higher-spin theories in AdS(5) gets enhanced, in a manner similar to that of AdS(3), to include additional generators that act on multi-particle states of the theory.



Publications

List of publications those form the thesis

1. Partition Functions for Higher-Spin theories in AdS. Rajesh Kumar Gupta, Shailesh Lal. JHEP 1207 (2012) 071, [arXiv:1205.1130]
2. One loop partition function for Topologically Massive Higher Spin Gravity. Arjun Bagchi, Shailesh Lal, Arunabha Saha, Bindusar Sahoo. JHEP 1112 (2011) 068, [arXiv:1107.2063] [arXiv:1107.2063]
3. The Heat Kernel on AdS. Rajesh Gopakumar, Rajesh Kumar Gupta, Shailesh Lal. JHEP 1111 (2011) 010 [arXiv:1103.3627]

List of papers those at are not included in the thesis

1. Topologically Massive Higher Spin Gravity. Arjun Bagchi, Shailesh Lal, Arunabha Saha, Bindusar Sahoo. JHEP 1110 (2011) 150, [arXiv:1107.0915]
2. Rational Terms in Theories with Matter. Shailesh Lal, Suvrat Raju. JHEP 1008 (2010) 022, [arXiv:1003.5264]
3. The Next-to-Simplest Quantum Field Theories. Shailesh Lal, Suvrat Raju. Phys. Rev. D81 (2010) 105002, [arXiv:0910.0930]



Name : **Tapas Chatterjee**
 Enrolment No. : MATH10200804005
 Constituent Institute : Institute of Mathematical Sciences, Chennai
 Title : Periodic Dirichlet Series and Transcendence

Abstract

In 1982, P. Chowla and S. Chowla stated a conjecture which says that $L(2, f) \neq 0$ except when

$$f(1) \equiv f(2) \equiv \dots \equiv f(p-1) = \frac{f(p)}{1-p^2}$$

A little later, Milnor put the conjecture of Chowlas' in a conceptual framework. He interpreted the conjecture of Chowlas' in terms of the values of the linear independence of the Hurwitz zeta function and conjectured that, for a prime p and integer $k > 1$, the $p-1$ real numbers

$$\zeta(k, 1/p), \zeta(k, 2/p), \dots, \zeta(k, (p-1)/p)$$

are linearly independent over \mathbb{Q} . In fact, Milnor suggested a generalization of this conjecture for arbitrary integer $q > 1$. This conjecture has been investigated in the recent works of Gun, Murty and Rath. Following their convention, for integers $k, q > 1$, let $V_k(q)$ denote the \mathbb{Q} -vector space generated by the numbers $\zeta(k, a/q)$ where a runs over the co-prime residue classes mod q . Then the conjecture of Milnor states that \mathbb{Q} -dimension of $V_k(q) \equiv \varphi(q)$. Gun, Murty and Rath proved that the above conjecture of Milnor is intimately linked to irrationality of $\zeta(k)$ for odd k . They derived a non-trivial lower bound for the dimension of $V_k(q)$, namely that

$$\mathbb{Q}\text{-dimension of } V_k(q) > \varphi(q)/2.$$

Further, the investigations carried out by them led them to formulate the following extension of the original conjecture of Milnor. More precisely, they conjecture that, in addition to Milnor's conjecture, the \mathbb{Q} -vector spaces $V_k(q)$ and \mathbb{Q} are linearly disjoint.

In other words, the \mathbb{Q} -vector space $V_k(q)$ generated by 1 and the Hurwitz zeta values $\zeta(k; a/q)$ for $(a, q) = 1$ has \mathbb{Q} -dimension $\varphi(q) + 1$.

As before, following Gun, Murty and Rath, we refer to this as the Strong Chowla-Milnor conjecture. In the first part of our thesis, we investigate various ramifications of this generalized conjecture. In many ways, this provides a more natural framework than the original conjecture of Milnor. Further, we formulate and investigate a number field analog of this conjecture. In the last part, we prove that there exist infinitely many zeros of certain generalized Hurwitz zeta functions in its half plane of absolute convergence. This can be thought of as a generalization of a classical problem of Davenport, Heilbronn and Cassels about the number of zeros of Hurwitz zeta function in the same half plane. We also investigate about zero-free region for such functions and prove a variant of a conjecture of Erdos.



Publications

1. Tapas Chatterjee, On The Dimension Of Chowla-Milnor Space, Proc. Indian Acad. Sci. Math. Sci., 122 (3), (2012), 313-317.
2. Tapas Chatterjee, The Strong Chowla-Milnor spaces and a conjecture of Gun, Murty and Rath, Int. J. Number Theory, 8(5), (2012), 1301- 1314.
3. Tapas Chatterjee and Sanoli Gun, Generalization of a problem of Davenport, Heilbronn and Cassels, submitted.
4. Tapas Chatterjee, Sanoli Gun and Purusottam Rath, Number _eld extension of a question of Milnor, in preparation.



Name : **Sachin S. Sharma**
Enrolment No. : MATH10201004001
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Title : They t-Analogue of String Functions for the Affine Kac-Moody Algebras

Abstract

We study Lusztig's t-analogue of weight multiplicities associated to the irreducible integrable highest weight modules of a_n Kac-Moody algebras. First, for the level one representation of twisted a_n Kac-Moody algebras, we obtain an explicit closed form expression for the corresponding t-string function using constant term identities of Macdonald and Cherednik. The closed form involves the generalised exponents of the graded pieces of the twisted affine algebra, considered as modules for the underlying finite dimensional simple Lie algebra. This extends previous work on level 1 t-string functions for the untwisted simply-laced affine Kac-Moody algebras. Next, for the Lie algebra $A_1^{(1)}$ we give a basis for the weight spaces of its basic representation, which is compatible with the a_n Brylinski-Kostant filtration defined by Slofstra. Using this basis we give an alternative derivation of the expression for the t-string function of the basic representation. Finally, we obtain explicit formula for the t-string function of irreducible integrable highest weight $A_1^{(1)}$ modules of all levels. This is generalisation of a theorem of a Kac and Peterson.

Publications

1. Sachin S. Sharma; Sankaran Viswanath; Suresh Govindarajan. A_n Brylinski- Kostant filtration on the basic representation of $A_1^{(1)}$ (pre-print).
2. Sachin S. Sharma; Sankaran Viswanath. The t-string functions of $A_1^{(1)}$ (pre-print).
3. Sachin S. Sharma; Sankaran Viswanath. The t-analog of the level one string function for twisted affine Kac-Moody algebras. C. R. Math. Acad. Sci. Paris 350 (2012), no. 3-4, 131-136.
4. Sachin S. Sharma; Sankaran Viswanath. The t-analog of the basic string function for twisted a_n Kac-Moody algebras. J. Algebra, 363:19-28, 2012



Name : **Vinayak C. Palve**
Enrolment No. : LIFE09200704001
Constituent Institute : Tata Memorial Centre, Parel, Mumbai
Title : Role of Anti-Apoptotic Mcl-1 Gene in Human Oral Cancers and Premalignant Lesions

Abstract

In the present work, the candidate has undertaken a multifaceted approach and studies the expression of Mcl-1 gene/splice variants in oral cancer cell lines, tumors and healthy tissues. Further, the contribution of high anti-apoptotic Mcl-1 expression was studied on radioresistance as well as chemoresistance of oral squamous carcinoma cells which is believed to flash light on the important mechanisms involved towards the treatment resistance in this cancer. Using several cutting edge technologies like RNAi knockdowns, the candidate has shown the significant role of Mcl-1L expression on cell survival and proliferation. His studies has shown, Mcl-1 to be an important pro-survival factor contributing to radio resistance & chemoresistance of oral squamous cell carcinomas. His studies not only showed high Mcl-1 expression in node positive and advanced tumors but also an important correlation between high expressions of Mcl-1 with poor overall survival of oral cancer patients. This indicates Mcl-1 expression to be an independent prognostic factor for oral cancer. In the field of oral cancer, the candidate has also studied effect of Mcl-1 genomic alterations, on its expression & treatment outcome cohort of oral cancer patients from Indian population. This study could be immensely useful in the treatment of radio & chemo resistant carcinomas with the help of certain BH3 mimetic inhibitors in order to achieve significant cell death at lower doses of chemotherapeutic drugs. Thus his studies suggest that Mcl-1L isoform has an important role in survival and radioresistance as well as chemoresistance of OSCC and may be a promising therapeutic target in oral cancer. The work has great significance as it addresses all the major factors contributing towards treatment resistance and outcome of oral cancer patients in Indian population.

Publications:

1. Vinayak C Palve and Tanuja R Teni, 'Association of anti-apoptotic Mcl-1L isoform expression with radioresistance of oral squamous carcinoma cells'. Radiation Oncology, Aug 8; 7:135, 2012.
2. S Mallick, R Patil, R Gyanchandani, S Pawar, V Palve et al., 'Human oral cancers have altered expression of Bcl-2 family members and increased expression of the antiapoptotic splice variant of Mcl-1'. Journal of Pathology, 217: 398- 407, 2009.



Name : **Rahul Checker**
Enrolment No. : LIFE01200804004
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Studies on the Perturbation of Immune System During Inflammation and its Modulation by Plumbagin

Abstract

While acute inflammation is an important element of the organism's defense repertoire, chronic inflammation can lead to several undesired side effects. Suppression of this unwanted and chronic activation of immune cells is desirable and can be achieved by inhibiting lymphocyte response pathways, depleting lymphocytes, or diverting lymphocyte traffic. The immunosuppressive regimens currently employed have distinct side effects on normal tissues which limits their long term usage. The objective remains to identify novel anti-inflammatory & immunosuppressive agents for treatment for while limiting the side effects. It is well known that transcription factor NF-kappaB is central to a series of cellular processes like inflammation, cell proliferation and apoptosis and is of particular importance in modulating the expression of immunoregulatory genes. Based on these observations, we speculated that plumbagin (a quinone found in the plants of Droseraceae, Plumbaginaceae, Anastrocladaceae and Dioncophyllaceae families), which was recently shown to inhibit constitutive as well as inducible NF-kappaB activation and NF-kappaB regulated genes in tumor cells, may show immunomodulatory effects and might have significant clinical application in prevention of inflammatory disorders. To test this hypothesis, the immunomodulatory effects of plumbagin were studied in murine lymphocytes in vitro and its in vivo anti-inflammatory efficacy was also investigated using mouse models of inflammatory disorders. Plumbagin inhibits mitogen induced lymphocyte cell activation, proliferation and cytokine secretion. Plumbagin also inhibits upregulation of activation markers and co-stimulatory molecules involved in T cell and B cell activation. Plumbagin modulated cellular redox status and acts via a novel redox dependent mechanism which is independent of ROS but dependent on GSH. Anti-inflammatory effects of plumbagin are mediated by inhibition of NF-kappaB and MAPKinase activation in lymphocytes. Plumbagin interacts with free thiol groups present on proteins and also induces protein S-glutathionylation in lymphocytes. Plumbagin (2mg/Kg body weight) administration to mice could prevent mortality and morbidity associated with graft-versus-host disease and septic shock. It was also able to significantly delay allograft rejection in mice model of allograft transplant. These results highlight a potential application of plumbagin as an immunosuppressive agent which may be used in the treatment of inflammatory disorders. This study also showed a ROS-independent mechanism of anti-inflammatory action of plumbagin. For the first time, evidence for a role for glutathionylation of cellular proteins as a mechanism of anti-proliferative action of plumbagin is provided. Further, mechanistic basis for potential therapeutic application of plumbagin as an immunosuppressive or anti-inflammatory drug is highlighted.

Publications

1. Checker Rahul, Sharma D, Sandur SK, Subrahmanyam G, Krishnan S, Poduval TB, Sainis KB. Plumbagin inhibits proliferative and inflammatory responses of T cells independent of ROS generation but by modulating intracellular thiols. *J Cell Biochem.* 2010 Aug 1;110(5):1082-93.
2. Checker Rahul, Sharma D, Sandur SK, Khanam S, Poduval TB. Antiinflammatory effects of plumbagin are mediated by inhibition of NF-kappaB activation in lymphocytes. *Int Immunopharmacol.* 2009 Jul;9(7-8):949-58.



Name : **Madhusmita Behera**
Enrolment No. : CHEM02200704012
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : A Study on High Temperature Phase Stability and Phase Transformation Characteristics in Ti-Ta and Ti-Ta-Nb Alloys Using Calorimetry and Microscopy Techniques

Abstract

Titanium and its alloys occupy a unique position in the world of engineering materials due to their wide range of applications in aerospace, petrochemical, biomedical and also in nuclear industry. Such versatile use of titanium alloys are owing to the combination of physical, chemical and processing characteristics, the latter being extremely important from the point of view of fabricating advanced engineering components and stronger structures that are expected to have good high temperature phase and microstructure stability, adequate corrosion resistance and excellent biocompatibility. The end application of any alloy can be met by tailoring the microstructure through thermo-mechanical and /or heat treatment which depends on the accurate thermo-kinetic data base. $\alpha + \beta$ or β titanium alloys containing refractory elements like Ta, Nb, Mo and Zr are challenging to process through standard and conventional routes in bulk quantities because the achievement of chemical homogeneity at the end of the treatment is difficult in these alloys due to sluggish diffusion of refractory elements. Hence, a complete understanding of the physical metallurgy, in particular the energetic and kinetics of both diffusional and displacive $\alpha \leftrightarrow \beta$ transformation is essential.

Hence, for the reasons stated above a fundamental investigation on high temperature thermodynamic and kinetic aspects of phase stability, especially with regard to $\alpha \leftrightarrow \beta$ phase transformation behaviors of Ti-xTa (x=5, 10,15 and 20 mass %) and Ti-5 mass% Ta-1.8 mass % Nb alloys has been carried out as a part of this thesis. For this purpose the isothermal drop calorimetry and high temperature differential scanning or dynamic calorimetry are use as the major experimental techniques, the results of which are supplemented by microstructural characterization of post calorimetry samples. The enthalpy increment ($H_T - H_{298.15}$) for four Ti-x Ta (x= 5,10,15,20 mass%) alloys are measured in the temperature range of 463 – 1257 K, which includes $\alpha + \beta$ phase field and also the $\alpha + \beta \rightarrow \beta$ phase change. The measured enthalpy variation in the transformation domain is used to obtain the energetic quantities of $\alpha + \beta \rightarrow \beta$ phase change and this is accomplished by invoking an appropriate description of the diffusional kinetics involved. The kinetics of thermally activated $\alpha \rightarrow \beta$ and $\beta \rightarrow \alpha$ phase transformation in Ti-5, 10, 15 and 20 Ta alloys is studied using dynamic calorimetric as a function of several scan rates in the range 3-99 K min⁻¹. The kinetics of phase transformation during heating and cooling has been modeled by KJMA (Kolmogorov-Johnson-Mehl-Avrami) formalism to estimate the kinetics parameters. Useful data on continuous heating transformation (CHT) and continuous cooling transformation (CCT) have been reported for all the four Ti-Ta binary alloys. Thermodynamics and kinetics of $\alpha \rightarrow \beta$ and $\beta \rightarrow \alpha$ phase transformation in Ti-5Ta-1.8Nb alloy are studied along the same line as that on Ti-Ta binary alloys. The mechanism of phase transformation on continuous cooling from the high temperature β phase is characterized using electron microscopy.

Publications

a. Journal

1. Madhusmita Behera, S. Raju, B. Jeyaganesh, R. Mythili, and S. Saroja, "A study on thermal properties and α (hcp) \rightarrow β (bcc) phase transformation energetics in Ti - 5 mass% Ta - 1.8 mass% Nb Alloy using inverse drop calorimetry", Int. J. Thermophys., 31 (2010) 2246-2263.



2. Madhusmita Behera, R. Mythili, S. Raju, and S. Saroja, "Effect of cooling rate on mechanism of $\beta \rightarrow \alpha$ phase transformation on continuous cooling in Ti-5Ta- 1.8Nb alloy", J. Alloys Compd., 553 (2013) 59-68.
3. Madhusmita Behera, S. Raju, Arun Kumar Rai, and S. Saroja, "Calorimetry investigation of phase stability and thermal property in Ti – 5 mass% Ta Alloy", DOI 10.1007/s12666-013-0250-1
4. Madhusmita Behera, S. Raju, R. Mythili, and S. Saroja, "High Temperature Drop Calorimetry Measurements of Enthalpy Increment in Ti-x Ta (X = 5, 10, 15, 20 mass %) Alloys" accepted in J Phy. Chem. solids 2013.
5. Madhusmita Behera, S. Raju, R. Mythili, and S. Saroja, "Kinetics of $\alpha \leftrightarrow \beta$ phase transformation in Ti- x Ta (X = 5, 10, 15, 20 mass %) alloys, communicate o J. Alloys Compd 2013.
6. Madhusmita Behera, R. Mythili, S. Raju, and S. Saroja, Characterization of $\alpha \leftarrow \beta$ phase transformation kinetics in Ti – 5 mass% Ta – 1.8 mass% Nb using Differential Scanning Calorimetry", to be communicated.

b. Conference Proceedings

1. Madhusmita Behera, B. Jeyaganesh, S. Raju, R. Mythili, Arun Kumar Rai and S.Saroja, "Drop calorimetry study on Ti – 5 wt% Ta – 1.8 wt% Nb alloy", Proceedings of the 17th DAE - BRNS National Symposium on Thermal Analysis, (THERMANS 2010), 46-48.
2. Madhusmita Behera, S. Raju, B. Jeyaganesh, R. Mythili, and S. Saroja, "A differential scanning calorimetry study of α (hcp) \leftrightarrow β (bcc) phase transformation kinetics in Ti - 5 wt.% Ta alloy", Proceedings of the International Symposium for Research Scholars, (ISRS- 2010), 243-246.

c. Conference Presentatio;ns

1. Madhusmita Behera, B. Jeya Ganesh, R. Mythili, S. Raju and S. Saroja, "A study of $\alpha \leftarrow \beta$ phase transformation in Ti - 5 wt. % Ta - 1.8 wt. % Nb alloy using Differential Scanning Calorimetry", presented in Structure and Thermodynamics of Emerging Materials (STEM- 2009).
2. Madhusmita Behera, B. Jeya Ganesh, R. Mythili, S. Raju and S. Saroja, "Phase transformation kinetics in Ti - 4.4 wt. % Ta - 1.8 wt. % Nb alloy using differential scanning calorimetry", presented in 63rd ATM, 16th – 17th November 2009, Science city, Kolkata.
3. Madhusmita Behera, R. Mythili, S. Raju and S. Saroja, "Study of $\beta \rightarrow \alpha$ Phase transformation on continuous cooling from the β phase field in a Ti-5%Ta- 1.8%Nb alloy" presented in 3rd National Symposium for Material Research Scholars, (MR10), 7-8th May 2010, IIT Bombay, Mumbai.
4. Madhusmita Behera, S. Raju, B. Jeyaganesh, R. Mythili, and S. Saroja, "Thermal stability and thermal property studies on Ti-5Ta & Ti - 5Ta-1.8Nb (mass%) alloy", presented in 19th European Conference on Thermophysical Properties (19 ECTP), 28th August – 1st September 2011, Thessaloniki, Greece.



5. Madhusmita Behera, S. Raju, Arun Kumar Rai and S. Saroja, "Calorimetric investigation of phase stability and thermal Property in Ti – 5 mass% Ta Alloy", presented in International Symposium for Research Scholars, (ISRS-2012), 13th - 15th December 2012, IIT Madras, Chennai, Tamil Nadu.

Related Work:

Journal

1. Josephine Prabha, S. Raju, B. Jeyaganesh, Arun Kumar Rai, Madhusmita Behera, M. Vijayalakshmi, G. Paneer Selvam and I. Johnson, "Thermodynamics of $\alpha \rightarrow \beta$ phase transformation and heat capacity measurements in Ti – 15 at % Nb alloy", Physica B, 406 (2011) 4200-4209.

Conference Proceedings

1. Josephine Prabha, S. Raju, B. Jeyaganesh, Arun Kumar Rai, Madhusmita Behera, M. Vijayalakshmi, and I. Johnson, "Drop Calorimetry characterization of a Ti-32.7 mass% Nb alloy having a significant amount of non-equilibrium β at room temperature", Proceedings of the International Symposium for Research Scholars, (ISRS- 2010), 62-65.



Name : **Kavita Garg**
Enrolment No. : CHEM01200804029
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Synthesis and Fabrication of Molecules for Molecular Electronic Devices and Sensors

Abstract

With the objective of using redox organic molecules to develop some organic electronics and sensor materials two σ - π - σ and two D-s-A systems were synthesized using unsymmetrical ABC₂ type porphyrins containing dialkylated *meso*-phenyl moieties, and β -alkenylamino TPP respectively. The monolayers, formed by electro-grafting these molecules on H-terminated Si surfaces were characterized. Evaluation of their electronic properties by *J-V* studies revealed room temperature NDR behavior by the σ - π - σ systems. The higher PVR (100at 1.09 V), observed with the device containing the fluoro-phenyl porphyrin moiety, compared to that (10 at 1.18 V) of its non-fluoro counter part may be due to its better organization by hydrogen bonding through the F atoms. The D-s-A- based monolayers showed current rectification in reverse bias with rectification ratio (RR) up to 10⁷. The high ionization energies and band gaps of perylenes/pyrenes n-type organic materials were utilized to construct σ - π systems-grafted Si hybrids that also showed good RR values. For this, the aromatic moieties were converted to some alkenylated derivatives that increased their solubility and assisted in covalent attachment to Si through the terminal olefin functionally.

For synthesizing the chemoresistive sensors, a bis-porphyrin (BP) along with its Zn²⁺- derivatives were synthesized, and spin-coated on glass surfaces. The thin films of BP showed reversible chemoresistive Cl₂ gas (10-500 ppb) sensing property at 170 °C, while both BP and Zn²⁺ - BP acted as selective and reversible room temperature NH₃ gas (1-20 ppm) sensors. The experimental results of electronics devices and sensors were explained by theoretical calculations.

Publications

1. K. Garg, A. Singh, A.K. Debnath, S.K. Nayak, S. Chattopadhyay, D.K. Aswal, Y. Hayakawa, S.K. Gupta, J.V. Yakhmi, *Bis-porphyrin films as ppb level chemiresistive sensors*. Chem. Phys. Lett. **2010**,488, 27–31.
2. K. Garg, A.Singh, C. Majumder, S. K. Nayak, D. K. Aswal, S. K. Gupta, S. Chattopadhyay. *Room temperature ammonia sensor based on jaw like bis-porphyrin molecules*. Organic electronics**2013**,14, 1021-1224

Communicated:

1. K. Garg, C. Majumder, S. K. Gupta, D. K. Aswal, S. K. Nayak, S. Chattopadhyay Stable Negative Differential Resistance in Porphyrin Based σ - π - σ Monolayers Grafted on Silicon. *J. Org. Chem*.
2. K. Garg, C. Majumder, S. K. Gupta, D. K. Aswal, S. K. Nayak, S. Chattopadhyay, Modulation of nanoelectronic behaviour porphyrin-silicon hybrid by changing the porphyrin substitution. *Org. Lett*.
3. K. Garg, C. Majumder, S. K. Gupta, D. K. Aswal, S. K. Nayak, S. Chattopadhyay Currentrectification behaviours of polyaromatic-monolayered silicon hybrids. *Org. Elec*.



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Enrolment No. : LIFE05200704003
Constituent Institute : Saha Institute of Nuclear Physics, Kolkata
Title : Characterization of Substrates of an S-Phase Cell Cycle Kinase of *Leishmania Donovan* with Emphasis on a Histone Acetyl Transferase

Abstract

The conserved family of cyclin dependent protein kinases (Cdks) primarily regulates the cell cycle progression in eukaryotes through phosphorylation of various key proteins. Several Cdk related kinases (CRKs) and cyclins have also been identified in early branching pathogenic kinetoplastida parasites *Leishmania*. An S-phase cell cycle kinase complex LdCyc1-CRK3 from *L. donovani* has been characterized previously in our lab. LdCyc1 contains a conserved MRAIL motif that is responsible for interaction with proteins harbouring R/KXL like Cyclin binding (Cy) motif. Since no knowledge about the identities of such targets of LdCyc1-CRK3 in *Leishmania* is available, a screen to identify substrates of the S-phase kinase was carried out based on the presence of Cy motif as well as Cdk phosphorylation site (S/T-P-X-R/K) on the targets. Three substrates of the cell cycle kinase could be identified, and among them, one is a unique protein with no known homologues. Another one is highly homologous to MYST family histone acetyl transferase (HAT). The third identified substrate is similar to DNA binding Ku-70 protein. All the identified substrates have been shown to be phosphorylated by LdCyc1-CRK3 through Cy-motif mediated association with the cyclin as shown by peptide competition and site directed mutagenesis studies (*FEBS Lett.* 2011, **585**:2635-39). Further characterization of the HAT homolog, termed as LdHAT1, has shown that it acetylates *L. donovani* histone H4 at K10 residue specifically, and interestingly, its activity is down-regulated after phosphorylation by LdCyc1-CRK3 (*FEMS Microbiol Lett.* 2012, **336**: 57-63). Since the homologous HAT from *Trypanosoma brucei* has been implicated in regulation of DNA replication, the result described here raised the possibility of a mode of regulation of replication through histone acetylation by a cyclin-Cdk. Therefore, the S-phase specific kinase LdCyc1-CRK3 may play an important role in S-phase related activities through the phosphorylation of LdHAT1 to control the cell cycle and life cycle of *L. donovani*.

Publications

1. Maity, A.K., Goswami, A., Saha, P. (2011) Identification of substrates of an S-phase cell cycle kinase from *Lishmania donovani*. *FEBS Letters*. 585, 2635–2639.
2. Maity, A.K., Saha, P. (2012) The histone acetyl transferase LdHAT1 from *Leishmania donovani* is regulated by S-phase cell cycle kinase. *FEMS Microbiology Letters*. 336, 57-63.



Name : **Sourabh Lahri**
Enrolment No. : PHYS07200604033
Constituent Institute : Institute of Physics, Bhubenswar
Title : Flutuation Relations, their Consequences and Some Examples

Abstract

In this thesis, we have studied some exact relations, called fluctuation relations, that are valid for systems that are perturbed arbitrarily out of equilibrium. These theorems include the Jazynski equality, Crooks fluctuation thermo, the total entropy production fluctuation theorems, the Hatano- Sasa relation, etc. We have studied the verification of some fluctuation theorem in different situations and model systems, and have put forward a few new ones. We have observed that Seifert's detailed fluctuation theorem for the total entropy change is valid even in the transient case for a system trapped in a harmonic potential, provided it begins from a state of thermal equilibrium. We have further observed that the two frequently used statements of the second law in terms of total entropy production and dissipated work, are not equivalent. A new quantifier of irreversibility of a process has been proposed. Several fluctuation theorems, both in classical and the quantum regime, have been extended to the case of feedback-driven systems. All the relations now are found to involve correction terms that depend on the way feedback is applied along the reverse process. In contrast, the second form of extended fluctuation theorems, that is expressed in terms of the so-called efficacy parameter, always retains the same form. The fluctuation theorems for total entropy change, work done and dissipated heat for a system in a time-periodic steady state, have been verified. In this case, a system present in a bistable potential has been considered, where the phenomenon of stochastic resonance has also been analyzed. Average work has been shown to be a better quantifier for stochastic resonance, than average total entropy change. In presence of biharmonic drive applied to the same system, particle confinement into one of the wells is obtained, along with a sharper stochastic resonance peak, in clear contrast to the behavior in presence of a static drive.

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2. * Entropy production theorems and some consequences, Arnab Saha, S. Lahiri and A. M. Jayannavar, Phys. Rev. E **80**, 011117 (2009).
3. * Energy fluctuations in a biharmonically driven nonlinear system. Navinder Singh, S. Lahiri, A. M. Jayannavar, Pramana J. Phys. **74**, 331 (2010).
4. Classical diamagnetism revisited, Arnab Saha, S. Lahiri and A. M. Jayannavar, Mod. Phys. Lett. B **24**, 2899 (2010).
5. Fluctuation theorems and atypical trajectories, Mamata Sahoo, S. Lahiri and A.M. Jayannavar, J. Phys. A: Math. Theor. **44**, 205001 (2011).
6. The role of soft versus hard bistable systems on stochastic resonance using average cycle energy as a quantifier, S. Rana, S. Lahiri and A. M. Jayannavar, Eur. Phys. J. B **84**, 323 (2011).
7. * Fluctuation theorems in presence of information gain and feedback, S. Lahiri, S. Rana and A. M. Jayannavar, J. Phys. A: Math. Theor. **45**, 065002 (2012).
8. Quantum Jarzynski Equality with multiple measurement and feedback for isolated system, S. Rana, S. Lahiri, A. M. Jayannavar, Pramana J. Phys. **79**, 233 (2012).



9. Fluctuation relations for heat engines in time-periodic steady states, S. Lahiri, S.
10. Rana and A. M. Jayannavar, J. Phys. A: Math. Theor. **45**, 465001 (2012).
11. Generalized entropy production fluctuation theorems for quantum systems, S. Rana, S. Lahiri and A. M. Jayannavar, Pramana J. Phys. **80**, 207 (2013).

Communicated

1. *Universal interpretation of efficacy parameter in perturbed nonequilibrium systems, S. Lahiri and A. M. Jayannavar, arxiv/cond-mat: 1206.3383.

(*) The starred publications are the ones on which the thesis is based.



Name : **Waikhom Sharatchandra Singh**
Enrolment No. : PHYS02200704005
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Optimization of GMR Array Sensor Based Magnetic Flux Leakage Techniques using Finite Element Modeling

Abstract

This thesis presents the three dimensional finite element (3D-FE) model based optimization of magnetic flux leakage (MFL) techniques for high sensitive, fast and reliable non-destructive detection of defects in ferromagnetic components of three different geometries viz. 1) cuboid geometry, 2) solid cylindrical geometry and 3) hollow cylindrical geometry. Carbon steel plates, track ropes of Heavy Water Plant (HWP) and steam generator (SG) tubes of Prototype Fast Breeder Reactor (PFBR) have been considered for cuboid, solid cylindrical and hollow cylindrical geometries, respectively. Experiments have been conducted to validate the model and to confirm the effectiveness of the model based optimization of the magnetizing units and giant magneto-resistive (GMR) sensor locations. Low-noise differential amplifiers and array sensors have been used for rapid imaging of defects.

Optimization of MFL technique for carbon steel plates (thickness, 12 mm) has been carried out by optimizing the leg spacing, height and magnetizing current of the electromagnetic yoke used in the technique. Optimised technique enabled successful detection of a sub-surface notch (depth, 0.9 mm) located at 11.1 mm below the surface. The MFL signal parameters namely, skewness and B_x - B_z locus patterns have been found to be useful for enhanced detection and classification of inclined and interacting defects.

MFL technique that uses saddle coils and GMR array sensors has been developed, for the first time, for inspection of track ropes (outer diameter, 64 mm) representing solid cylindrical geometry. A magnetizing current of 5 A and inter-coil spacing of the saddle coils of 75 mm have been found to be optimum using the model. The experimental results clearly confirmed the reliable detection of localized flaw (2 mm deep) and loss of metallic area (LMA) type defect (3 mm deep) in the track rope. Further, a novel flexible 12 element GMR array sensor has been developed and successfully used for rapid imaging of defects.

For MFL testing of SG tubes (outer diameter, 17.2 mm and wall thickness, 2.3 mm), the magnetisation unit comprising of two bobbin coils wound on a guided ferrite core has been optimized. The number of GMR sensors and their locations have been optimized by predicting the uniform magnetic flux density region between the two bobbin coils. A 5-element GMR array sensor has been fabricated and the performance of the GMR array sensor has been evaluated. Successful detection and imaging of 1 mm diameter localized hole in the tube has been achieved. The influence of Inconel support plate and sodium deposits on the outer surface of the tube on MFL signals has been analysed using the FE model.

This thesis has finally proposed a generalized approach for optimization of MFL techniques using finite element modeling for enhanced detection and fast imaging of defects in ferromagnetic components, without the need for extensive physical testing.



Publications

Journal

1. W. Sharatchandra Singh, B. P. C. Rao, S. Thirunavukkarasu, C. K. Mukhopadhyay and T. Jayakumar, "Design and optimization of GMR array based magnetic flux leakage probe for imaging of defects in small diameter steam generator tubes", *Sensors and Actuators A (Communicated)*.
2. W. Sharatchandra Singh, B. P. C. Rao, S. Thirunavukkarasu, C. K. Mukhopadhyay and T. Jayakumar, "GMR based magnetic flux leakage technique for detection of localized outer side defects in small diameter ferromagnetic steam generator tubes", *IEEE Transactions on Magnetics (Communicated)*.
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6. W. Sharatchandra Singh, B. P. C. Rao, S. Mahadevan, T. Jayakumar and Baldev Raj, "Giant magneto-resistive sensor based magnetic flux leakage technique for inspection of track ropes", *Studies in Applied Electromagnetics and Mechanics, Electromagnetic Nondestructive Evaluation (XIV)*, vol. 35, pp. 256-263, June 2011.
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1. W. Sharatchandra Singh, B. P. C. Rao, C. K. Mukhopadhyay and T. Jayakumar, "Giant magneto-resistive sensor array for non-destructive detection of leakage magnetic flux from surface defects in ferromagnetic materials", *International Conference On Sensors and Related Networks (SENNET 12)*, VIT University, India, pp. 71-73, January 2012.
2. W. Sharatchandra Singh, S. Thirunavukkarasu, S. Mahadevan, B. P. C. Rao, C. K. Mukhopadhyay and T. Jayakumar, "Three-dimensional finite element modeling of magnetic flux leakage technique for detection of defects in carbon steel plates", *Proc. of COMSOL Conference-2010*, Bangalore, India, October 2010 (CD released).
3. W. Sharatchandra Singh, K. Krishna Nand, B. P. C. Rao, T. Jayakumar and Baldev Raj, "Magnetic flux leakage NDE using giant magneto-resistive sensors", *Review of Progress in Quantitative NDE*, AIP Press, vol. 27B, pp. 857-864, March 2008.
4. W. Sharatchandra Singh, B. P. C. Rao, B. Sasi, S. Vaidyanathan, T. Jayakumar and Baldev Raj, "Giant magneto-resistive sensors for non-destructive detection of magnetic flux leakage from sub-surface defects in steels", *International Conference On Sensors and Related Networks (SENNET 07)*, VIT University, India, pp. 11-14, December 2007.



Name : **Namita Maiti**
Enrolment No. : ENGG01200704027
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Process Control of Electron Beam Systems for Thin Film Coating

Abstract

The process control of EBPVD based coating system is highly dependent on the performance of each subsystem of the EBPVD system. Though the electron gun technology has been evolving over the last few decades, there are several distinct specialized areas which require systematic investigation of electron gun. This work incrementally adds features in hardware meant for EBPVD and produces desirable results not possible without these additions. These are outlined as (a) design of high power electron gun which is suitable for high power evaporation system, (b) unhindered operation of the electron gun for nonmetallic coating to operate in an ambient of 10^{-1} Pa to 10^{-2} Pa so that stoichiometry issue can be tackled, (c) mechanism to protect high power source from breakdown to enable uninterrupted operation of electron gun, and (d) finally, we validate the effectiveness of the stoichiometry control through experimentation and characterization of a representative coating.

The electron gun plays the most important role, therefore in this work the major emphasis is on the design of the electron gun. Electron beam evaporation system is generally 270° bent beam type. Depending on the application the system is either high power type or low power type. For high power gun, the contribution in this thesis has been on an emitter design which overcomes the shortcomings of directly heated filament. The emission from directly heated cathode suffers due to cathode distortion and self-induced magnetic fields resulting in non-uniform distribution of heat flux on the work surface. In this direction the contribution has been on design of an indirectly heated cathode that provides longer cathode life and uniform temperature distribution over the cathode emitting area of interest.

In the low power regime, there has been significant contributions by various researchers. In this thesis, the emphasis has been given on gun design for reactive evaporation, which is carried out in the pressure range between 10^{-1} Pa to 10^{-2} Pa. At this high pressure the electron gun does not operate reliably due to high voltage flashover. To overcome this problem substrate chamber is isolated from gun chamber using a bifurcation plate. Using the differential pumping arrangement the gun chamber pressure is maintained at better than 5×10^{-3} Pa, whereas substrate chamber pressure is in the range between 10^{-1} Pa to 10^{-2} Pa. The coating experiment of alumina is carried out as reactive evaporation. Evaporation of alumina results in dissociation and loss of oxygen and hence reactive evaporation under oxygen-ambient has been carried out to compensate the oxygen loss. Pure (better than 99.9 %) quality oxygen gas (O_2) has been bled in the system during deposition and films have been deposited at various oxygen flow rates. Variations of the different properties of the Al_2O_3 films have been studied as a function of O_2 flow rate. This study was to obtain the optimum oxygen flow rate or partial pressure to achieve good quality films with reasonably high refractive index.

The design of the electron gun to reduce process interruptions due to breakdown has been taken up. Besides process degradation, this phenomena poses threat to the feeding power source and associated control electronics. In this thesis, ferrite beads have been used on both the feed cables to attenuate the breakdown current near the gun so that it does not propagate to the power source to cause any detrimental effect. The use of ferrite beads in both the conductors, as used in this work, offers attenuation to both common mode and also differential mode noise signals. The ferrite beads have



been used to suppress the high frequency content through dissipation and also to reduce the amplitude of the breakdown signal. Using the ferrite bead DC passes fully, but rejects best between 1-10 MHz and somewhat lesser extent a decade above and a decade below. Ferrites in this work act like a broadband reject filter without a sharp cut off.

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1. Namita Maiti, S. Mukherjee, Bhunesh Kumar, U. D. Barve, V. B. Suryawanshi, and A. K. Das, "Design and development of indirectly heated solid cathode for strip type electron gun", Review of Scientific Instruments, vol.81, no.1, pp.013302-013302-10, Jan 2010 doi: 10.1063/1.3271539
2. Namita Maiti, A. Biswas, R. B. Tokas, D. Bhattacharyya, S. N. Jha, U. P. Deshpande, U. D. Barve, M. S. Bhatia and A. K. Das, "Effects of Oxygen flow rate on microstructure and optical properties of Aluminum oxide films deposited by electron beam evaporation technique", Vacuum, Volume 85, Issue 2, 20 August 2010, Pages 214-220, ISSN 0042-207X, 10.1016/j.vacuum.2010.05.017.
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4. Namita Maiti, U. D. Barve, M. S. Bhatia, and A. K. Das, "Design of transverse electron gun for electron beam based reactive evaporation system", Review of Scientific Instruments, Review of Scientific Instruments, vol.82, no.5, pp.056106-056106-3, May (2011) doi: 10.1063/1.3597576
5. Namita Maiti, U. D. Barve, Shakti Kumar Mishra, M. S. Bhatia, and A. K. Das "Attenuation of electron gun generated surges in an electron beam evaporation system using ferrite beads", Vacuum, 86 (2012), pp 1810 - 1814, Available online 27 April 2012, ISSN 0042-207X, 10.1016/j.vacuum.2012.04.028.

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1. Namita Maiti, Atul Tak, Yashodhan Khabade, V. B. Suryawanshi and A. K. Das, "Modeling of vapor transport of electron beam evaporation based coating system", AIP Conf. Proc. 1451, (2012) pp 304-306.
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3. Pallab Karmakar, Namita Maiti, A V Bapat, "Design and Performance of Differential Pumping System of Coating Unit", International Symposium on "Vacuum Science and Technology", Journal of Physics: Conference Series 114 (2008) 012069.
4. Namita Maiti, P. Karmakar, U. D. Barve, A V Bapat, "An Evaporation System for Film Deposition Using Electron Beam Sources", International Symposium on "Vacuum Science and Technology", Bulletin of Indian Vacuum Society, Vol. 12(2), 2009, pp 3-7.
5. Namita Maiti, U.D. Barve, Jagannath, S.Mukherjee, M.S. Bhatia, A.K. Das, "Deposition of boron thin film by using electron beam evaporation technique", presented at National Conference on Recent Advances in Surface Engineering (RASE 09), National Aerospace Laboratories, Bangalore, 26-27 Feb'2009.



Name : **Maneesha Mishra**
Enrolment No. : CHEM02200804001
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Studies of Microstructures, Optical, Nanomechanical and Thermal Expansion Properties of Y_2O_3 , ZrO_2 , CeO_2 , and Gd_2O_3 Thin Films and Y_2O_3/ZrO_2 and CeO_2/Gd_2O_3 Multilayers Prepared by Pulsed Laser Deposition

Abstract

Metal oxides are important candidate materials in almost all domestic as well as industrial applications. Properties of materials can be tailored by changing the microstructure of materials, which are dependent on the process parameters of deposition techniques. This work consists of preparation of single layers of Y_2O_3 , ZrO_2 , CeO_2 and Gd_2O_3 , and multilayers structures of Y_2O_3/ZrO_2 , CeO_2/Gd_2O_3 by pulsed laser deposition technique, followed by characterization by conventional and high temperature X-ray diffraction, X-ray reflectivity, Raman spectroscopy, atomic force microscopy, high resolution transmission electron microscopy, UV-Visible spectroscopy and nanoindentation.

Y_2O_3 and ZrO_2 films were prepared on Si (100) and quartz substrates to study the effect of process parameters on the microstructural and optical properties. Multilayer structures of ZrO_2/Y_2O_3 were prepared at 300 and 873 K, followed by the measurements of optical and nanomechanical properties. All the films showed good transmittance in the wavelength range of 200-800 nm. Hardness values did not show any significant changes with ZrO_2 layer thickness. The coefficient of thermal expansion (CTE) values was calculated for single as well as multilayers of ZrO_2 and Y_2O_3 from HTXRD analysis. CTE multilayers were higher than that of the single layers, which is due to the interdiffusion effects.

CeO_2 and Gd_2O_3 single layers were prepared at different process parameters. CeO_2 films were crystallized with cubic structure and showed good transmittance in 200-800 nm. Gd_2O_3 films deposited at different substrate temperature and oxygen partial pressure showed mostly monoclinic peaks, along with small fraction of cubic Gd_2O_3 . CeO_2/Gd_2O_3 multilayers were deposited at 300 K and 873K at oxygen partial pressure of 2 Pa and showed better crystalline films formed at higher substrate temperature. Films showed good transmittance within wavelength range of 200- 822 nm. Hardness values obtained for CeO_2/Gd_2O_3 multilayers showed higher values than that of the hardness of single layers of CeO_2 and Gd_2O_3 . Coefficients of thermal expansion (CTE) values were calculated for the single as well as multilayer structures from the HTXRD data. And it was observed that the CTE values of CeO_2 and Gd_2O_3 were higher in multilayer structures than that of the single layers.

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2. "Phase Evolution in Zirconia Thin Films Prepared by Pulsed Laser Deposition" Maneesha Mishra, P. Kuppusami, A. Singh, S. Ramya, V. Sivasubramanian, E. Mohandas, Appl. Surf. Sci. 258 (2012) 5157.
3. "Microstructural and Optical Characterization Of ZrO_2/Y_2O_3 Multilayers Prepared by Pulsed Laser Deposition" Maneesha Mishra, P. Kuppusami, V. R. Reddy, A. Singh, G. Chinnamma, C. Ghosh, R.



Divakar, E. Mohandas. (Accepted in J. NanoSci. Lett. (2013) 3:4).

4. "Structural and optical properties of $\text{CeO}_2/\text{Gd}_2\text{O}_3$ multilayer structures prepared by pulsed laser deposition". M. Mishra, P. Kuppusami, V. R. Reddy, C. Ghosh, R. Divakar, E. Mohandas. (Manuscript under Review: Surface and Coating Technology).
5. "Stability of $\text{ZrO}_2/\text{Y}_2\text{O}_3$ multilayer structures By HTXRD". M. Mishra, P. Kuppusami, A. Singh, S. Murugesan, R. Thirumurugesan, E. Mohandas. (To be submitted to Materials Chemistry and Physics).
6. "Study of Thermal Stability of $\text{CeO}_2/\text{Gd}_2\text{O}_3$ multilayers prepared using pulsed laser deposition". M. Mishra, P. Kuppusami, A. Singh, R. Thirumurugesan, E. Mohandas. (To be communicated to J. Alloys and Compounds).
7. "Study of structural and optical properties of Gd_2O_3 thin films as a function of oxygen partial pressure". M. Mishra, P. Kuppusami, A. Singh, R. Thirumurugesan, E. Mohandas (To be communicated to Thin Solid Films).



Name : **Shashi Chandra Lal Srivastava**
Enrolment No. : PHYS04201004001
Constituent Institute : Variable Energy Cyclotron Centre, Kolkata
Title : Spectral Statistics, Random Matrix Theory, and Classification of Dynamical Systems

Abstract

Random matrix theory (RMT) has been developed for both Hermitian and pseudo-Hermitian systems with varying degree of success. In modern days, it has found applications in a variety of areas from basic sciences (Nuclear physics, Quantum Chaos, Number theory) to more applied areas like RNA folding in biology, wireless communication theory and financial analysis. In this thesis, we have developed RMT for pseudo-Hermitian systems and structures matrices, alongwith developing new measures like Stochasticity parameter and record statistics for classifying and characterizing dynamical systems quantum mechanically.

RMT has been extended for a structured class of matrices namely cyclic matrices, which form an example of pseudo-Hermitian systems. The joint probability distribution function for general N -dimensional matrices and hence all the correlation functions have been obtained analytically. These results have been utilized to solve the entropy evolution in case of biased random walks on disordered lattices and shown to saturate as expected to $\log N$. Importantly, the rate of approach to equilibrium for ensemble averaged jump probabilities has been shown to follow a $1/t$ law. The JPDF and all the spacing distribution etc have further been obtained for cyclic block matrices which are a general case of cyclic matrices. RMT has also been extended for another structured class of matrices, reverse cyclic matrices. These are a subset of symmetric matrices and shown to have an unusual density and spacing distribution. In contrast to the semi-circle density, this ensemble admits a density with a hole at the origin. Again, the spacing distribution has a variety, ranging from Gaussian-looking distributions to Wigner type distributions. Along with bulk properties like density, the record statistics of eigenvalues have also been obtained. Largest eigenvalue distribution is shown to be Gumbel. Corresponding to this class of matrices, associated exactly solvable many-body Hamiltonian in one dimension is the screened harmonic oscillator potential. All the findings have been corroborated by necessary numerical calculations.

Two new measures, record statistics and Stochasticity parameter have been proposed to characterize and classify the dynamical systems quantum mechanically. The record statistics for Intensity vectors of quantized standard map captures the transition from Integrable to mixed to chaotic regimes as a function of chaos parameter, K . The necessary generalizations of record statistics from independent and identically distributed systems to weakly correlated systems have been done. The Stochasticity parameter has been proposed and calculated for eigenvalues of various dynamical systems, ranging from circle, to triangle to standard map and Riemann zeroes. It has been shown that probability density function of Stochasticity parameter for Integrable and chaotic systems are distinctly different. The Stochasticity parameter itself scales as a power law with the number of eigenvalues and has been understood in terms of record statistics. A graph in terms of PDF evaluated at last member of sequence considered and scaling exponent of Stochasticity parameter put Integrable and chaotic systems on two different regions and paves the way to classify quantum mechanically the classically chaotic systems and Integrable systems.



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1. Published:

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3. "Random matrix theory for pseudo-Hermitian systems: Cyclic blocks", Sudhir R. Jain and Shashi C. L. Srivastava, Pramana J. Phys. 73, 989 (2009).
4. "Biased random walks on a disordered one-dimensional lattice", K. Manikandan, Shashi C. L. Srivastava, Sudhir R. Jain. Phys. Lett. A 375, 368 (2011).
5. "Random reverse-cyclic matrices and screened harmonic oscillator", Shashi C. L. Srivastava and Sudhir R. Jain, Phys Rev E 85, 041143 (2012).
6. "Pseudo-Hermitian random matrix theory", Shashi C. L. Srivastava and Sudhir R. Jain, Fortschr. Phys., 61, 276 (2013).
7. "Record statistics in random vectors and quantum chaos", Shashi C. L. Srivastava, Arul Lakshminarayan, Sudhir R. Jain, EPL (Europhysics Letters) 101, 10003 (2013).

2. Unpublished:

1. "Kolmogorov stochasticity parameter as a measure of quantum chaos",
2. Shashi C. L. Srivastava and Sudhir R. Jain, arXiv:1101.5465



Name : **Anoop Varghese**
Enrolment No. : PHYS10200604015
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Phase Transitions in Polyelectrolyte Systems

Abstract

In this thesis, we study the phase behaviour of three different polyelectrolyte systems. The first system is a single flexible polyelectrolyte, for which we identify the counterion condensation as a second-order phase transition, and counterions mediated collapse of the polyelectrolyte chain as a first-order phase transition. We also show that the critical value of the linear charge density of the polyelectrolyte chain for both transitions decreases with increasing valency of the counterions. The second polyelectrolyte system that we have considered is a system of rod-like polyelectrolytes. We show, in contrast to earlier simulation and theoretical studies, that monovalent counterions mediate aggregation of similarly charged rod-like polyelectrolyte chains. We also show that the critical value of the linear charge density for the aggregation coincides with that for counterions mediated collapse of a single flexible polyelectrolyte chains, suggesting that the underlying mechanism for both transitions are related. The third system that has been considered is a two-dimensional system of a charged disc and counterions. We calculate the microcanonical entropy of this system exactly and compare the thermodynamics of the system derived from the canonical partition function. We show that the microcanonical entropy is concave, and as a result, the canonical and microcanonical ensembles are equivalent, even though the interactions in the system are long-ranged.

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2. Ensemble Equivalence for Counterion Condensation on a Two Dimensional Charged Disc, A. Varghese, S. Vemparala and R. Rajesh, Phys. Rev. E 85, 011119 (2012)
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4. Aggregation of Rod-like Polyelectrolyte Chains in the Presence of Monovalent Counterions, A. Varghese, R. Rajesh and S. Vemparala, J. Chem. Phys. 137, 234901 (2012)



Name : **Ujjwal Sinha**
Enrolment No. : PHYS06200704014
Constituent Institute : Institute for Plasma Research, Gandhinagar
Title : Radiation Pressure Acceleration of Ions in Bulk Targets by Ultra-Intense Laser Pulses

Abstract

The present thesis examines some important issues regarding acceleration of plasma ions to high energies by ultra-intense circularly polarized (CP) lasers in the Hole Boring (HB) mode of Radiation Pressure Acceleration (RPA). A major part of the study is devoted to the analysis of the accelerating structure (laser piston) under the influence of a longitudinal magnetic field as well as for a plasma target composed of multiple ion species. The laser piston is a charge separation layer created due to the ponderomotive force of the incident laser. This induced charge separation field is responsible for accelerating the plasma ions. Under the influence of a static magnetic field, the polarization state (i.e. left or right circulation) plays an important role in this process. It has been found that right circularly polarized (RCP) lasers are more efficient as the net ponderomotive force on plasma electrons is enhanced in this case due to resonance between their quiver motion in laser field and cyclotron motion due to applied magnetic field. Further a residual ion space charge behind the laser piston is discovered. It is found that this space charge undergoes coulomb explosion under its own field and does not contribute to the accelerated ion beam. However when an energetic test ion is incident in the direction opposite to the incident laser, this coulomb exploding region reflects it with a velocity higher than the incident velocity, thus amplifying the kinetic energy of the test ion.

Further acceleration of ions using ultra-intense laser irradiated on an overdense target plasma composed of two ion species has been described using a self-consistent approach. The analytical model for the steady state described here gives a complete description of the charge separation zone, i.e., ion space charge and electron sheath, created due to ponderomotive force of the laser. It successfully explains the jump in electrostatic potential or field in the laser piston responsible for a major part of the acceleration. The information about the structure of laser piston obtained from the analytical model is used for the stability analysis of the process. It has been found that the stability of the laser piston depends on the target composition. The reflection of incoming test ion from the coulomb exploding region of the ion space charge has been described in context of the charge on the incident beam species.

Extending the theory of ion acceleration to two dimensions (i.e. radial and axial with azimuthal symmetry), it was found that a radial intensity variation in the incident circularly polarized (CP) laser introduced radial electron density inhomogeneity in the electron sheath formed due to ponderomotive pressure. This density inhomogeneity drives an azimuthal current. Besides this the circular motion of the plasma electrons under the influence of the CP laser field induces a magnetic dipole moment. This dipole moment when summed over all the plasma electrons gives rise to a net magnetization. The azimuthal and magnetization current together generates a quasi-static axial magnetic field in the mega-gauss regime.

Finally the multi-stage process of ion acceleration is studied in the relativistic regime. A fully relativistic calculation for the second stage ion velocity is presented and is validated using 1D3V particle in cell (PIC) simulations. Also a comparative study between non-relativistic and relativistic case is done and it is found that at high piston velocities the relativistic results differ a lot from the non-relativistic ones.



Publications

1. Ujjwal Sinha and Predhiman Kaw, "Ponderomotive Ion Acceleration in dense magnetized laser irradiated thick target plasmas", Physics of Plasmas 19, 033102(2012)
2. Ujjwal Sinha, "Self Consistent model for ponderomotive ion acceleration of laser irradiated two species dense target plasmas", Physics of Plasmas 19, 043104(2012)
3. Ujjwal Sinha, "Multistage Ion Acceleration in Finite Overdense Target with a Relativistic Laser Pulse", Physics of Plasmas 20, 073116(2013)
4. Ujjwal Sinha and Predhiman Kaw, "Analytical model for axial magnetic field generation by interaction of radially inhomogeneous laser pulse with a solid target", (to be submitted)



Name : **Jaya Maji**
Enrolment No. : PHYS07200804001
Constituent Institute : Institute of Physics, Bhubaneswar
Title : Effimov-Like States and Conformational Transitions of DNA

Abstract

In this thesis we have studied the melting of a triple-stranded DNA and the conformational transitions of a double-stranded DNA from the B form to the Z form.

Certain sequences of Watson-Crick-dsDNA allow a third strand DNA to bind via Hoogsteen or reverse-Hoogsteen base pairing to form a tsDNA. The formation of a triple helical DNA is of great interest in current era. Owing to its enhanced stability in affecting the activities such as gene expression, DNA replication and others requiring DNA opening, the triple helix fostered new hopes in therapeutic applications.

The existence of an Efimov like state, where not two are bound but an effective three chain bound state, has been shown for three strands of DNA using a hierarchical lattice model of dimensions $d > 2$. Such a state can occur at or above the duplex melting point and the phenomenon is analogous to the Efimov state in three-particle quantum mechanics. We also show that a transition can be induced from the Efimov DNA to a critical state if the three chain system is treated in a higher dimensional lattice. Real space renormalization group (RG) and exact numerical calculations are used. The feature of enhanced stability of triple helix compared to the duplex-DNA is obtained by these numerical calculations.

The melting of triple stranded DNA has also been studied in lower dimensional Sierpinski gasket lattice models ($d < 2$). In presence of some extra weight factors the phase diagram of a triple-stranded DNA is obtained for different models. We verify the the Efimov DNA does exist, but under different conditions a thermodynamically stable state appears. We call it a mixed state, where the strands are pair-wise bound but no three chain contacts. All these transitions are induced by the bubble formations.

Melting or unzipping are considered to be the crucial step in many biological processes such as DNA replication, conformational transition and RNA transcription etc. Though B is the most common form of DNA under normal physiological conditions, under certain circumstances a conformational transformation from B to the Z form takes place. The dynamic phase diagram is obtained for the stability of the front separating B and Z. The instability in this front results in two split fronts moving with different velocities. Hence, depending on the system parameters a denatured state may develop dynamically even though it is thermodynamically forbidden.

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1. Jaya Maji and S.M. Bhattacharjee, Euro Phys. Letts. 81, 30005 (2008), Nonequilibrium tricriticality in one dimension.
2. * Jaya Maji, S.M. Bhattacharjee, F. Seno, and A. Trovato, New J. Phys 12, 083057 (2010) , When a DNA triple helix melts; an analogue of the Elimov state
3. * Jaya Maji and S.M. Bhattacharjee, Euro Phys. Letts. 92, 58004 (2010), Dynamic phase transition in the conversion of B-DNA to Z-DNA.



4. P. Sadhukhan, Jaya Maji and S.M. Bhattacharjee, Euro Phys. Letts., 95, 48009 (2011), Type II DNA: When the interfacial energy becomes negative.
5. * Jaya Maji and S.M. Bhattacharjee, Phys. Rev. E86, 041147 (2012), Efimov effect of triple stranded DNA: Real Space Renormalization Group and Zeros of partition function.
6. * Jaya Maji, S.M. Bhattacharjee, F. Seno, and A. Trovato, arXiv: 1306, 4206, Strange phases in three stranded DNA-models at low dimensionality.

(*) indicates the papers on which this thesis is based.



Name : **Shankhadeep Chakrabortty**
Enrolment No. : PHYS07200604032
Constituent Institute : Institute of Physics, Bhubaneswar
Title : Aspects of Gauge/Gravity Duality

Abstract

Gauge/gravity duality provides a systematic prescription to explore some strongly theories. On one hand, by exploring strong/weak nature of this duality, we can uncover features of the strongly coupled gauge theories by studying the dual weakly coupled gravity. On the other hand, physics of the non-perturbative string/M theory becomes accessible by analyzing weakly coupled boundary duals. The thesis attempts explore both sides of this duality. While studying the strong coupling limit of gauge theory. We focused on a holographic QCD model and the quark cloud model which is the $N = 4$ SYM plasma at finite temperature with additional heavy fundamental static quarks. We use the holographic techniques to calculate the drag force, jet quenching parameter and screening length of the quark and the antiquark. These quantities are sensitive to the strong coupling nature of gauge theory in the context of quark gluon plasma.

In the case of holographic QCD model, we found that when the chemical potential is higher than a critical value, the drag force increases with temperature while the Jet quenching parameter monotonically decreases with the temperature. Below this critical value of the chemical potential, we have found both of the drag force and jet quenching parameters behave as multivalued functions of temperature and this behavior is consistent with the existence of the first order phase transition in this hQCD model. More over it becomes evident from our study that the quark antiquark pair dissociates beyond a characteristic screening length of the system.

In the second part of the thesis, we explored the strong coupling side of the string/M theory via the analysis in the dual weakly coupled field theory. In particular, by exploiting the AdS₄/CFT₃ correspondence, we studied a class of semiclassical, nonperturbative objects in gravity theory known as the giant graviton and the dual giant graviton. These objects are either spherical M-2/M-5 branes living in AdS₄ × S⁷/Z_k geometry or spherical D-2/ D-4 branes living in AdS₄ × CP₃ geometry. Using the operator state correspondence prescribed by the AdS₄/CFT₃ dictionary, we mapped these gravity states in to the ½ BPS gauge invariant chiral primary operators in the dual weakly coupled N= 6, U (N₁) × U (N₂) ABJ (Aharony, Bergman, Jafferis) gauge theory. We showed the correct gauge invariant operators dual to the giants with large angular momentum are the Schur polynomial operators with the large R Charges. Using the combinatorics of Young tableaux representation of these Schur polynomials, we calculated the various gauge theory correlators representing transitions among the giants. In the N₁ = N₂ limit ABJ theory, there is an alternative world volume theory of multiple M-2 branes known as BLG (Bagger, Lambert, Gustavson) theory. Motivated by the importance of 3 – algebraic structure in this BLG theory we constructed a novel 3 – algebra consisted of w_{∞} generators.

Publications

1. **Some aspects of QGP phase in a hQCD model*”, R. G. Cai, S. He and Li.Li and Shankhadeep Chakrabortty, arXiv:1209.4512 [hep-th].



2. **“Correlators of Giant Gravitons from dual ABJ(M) Theory”*, T. K. Dey and Shankhadeep Chakrabortty, JHEP 1203, 062 (2012), arXiv:1112.6299 [hep-th].
3. * *“Dissipative force on an external quark in heavy quark cloud”*, Shankhadeep Chakrabortty, Phys. Lett. B 705, 244 (2011), arXiv:1108.0165 [hep-th].
4. *“Some BPS configurations of the BLG Theory”*, S. P. Chowdhury, K. Ray and Shankhadeep Chakrabortty, Phys. Lett. B 703, 172 (2011), arXiv:1105.2898 [hep-th].
5. *“Moduli and BPS configurations of the BLG theory”*, S. P. Chowdhury, T. Koppe, K. Ray and Shankhadeep Chakrabortty, Phys. Lett. B 695, 285 (2011), arXiv:1005.3707 [hep-th].
6. *“Proof of universality of electrical conductivity at finite chemical potential”*, Sayan K. Chakrabarti, Sachin Jain, Shankhadeep Chakrabortty, JHEP 1102, 073 (2011) arXiv:1011.3499 [hep-th].
7. **“ w_1 3-algebra ”*, Alok Kumar, Sachin Jain and Shankhadeep Chakrabortty, JHEP 0809:091, (2008), arXiv:0807.0284 [hep-th].

(*) indicates papers on which this thesis is based.



Name : **Sunil Rawat**
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Title : Behaviour of Solids Under High Strain-Rate Deformation

Abstract

Solid fracture under high strain-rate deformation is of interest for high velocity impact and penetration problems. Hydrodynamic simulations are widely used to study the material deformation and fracture. The main inputs to hydrodynamic simulations are (a) fracture model such as void Nucleation and Growth (NAG) model (b) material strength model such as Johnson-Cook model (c) equation of state (EOS) such as the Murnaghan EOS. The above models involve several parameters. For example, the NAG model involves several parameters: void nucleation threshold, void growth threshold, pressure sensitivity, material viscosity and nucleation rate at threshold. In the literature, the parameters for these models are available only for a few materials. Therefore, for predictive simulations it is necessary to generate these parameters for different materials of interest to DAE either by experiments or by first principle/atomistic simulations.

High strain-rate phenomenon like plate impact experiments at few hundred m/s involves compressive stress waves at the point of impact. These waves reach the free surfaces of the projectile and target and reflect as release waves. The interaction of release waves leads to tensile pressure in the material. During this process, there is a transition from uniaxial state of strain to triaxial state. If the tension created exceeds the tensile strength of the material, nucleation, growth and coalescence of the voids occur leading to fracture. This process has been simulated using classical molecular dynamics in which a solid is triaxially deformed at high strain rate till the nucleation, growth and coalescence of voids occur. The highlights of the simulations for fracture properties are:

1. A method to obtain NAG parameters using large-scale atomistic simulations is developed.
2. The NAG parameters have been obtained for perfect single crystal copper. The void nucleation threshold obtained matches with the spall strength obtained in laser driven spall experiments on micron sized copper foils. Since perfect single crystals are not available, they have been validated by molecular dynamics simulations of high velocity impact induced spallation of perfect single crystal copper.
3. The effect of temperature on the NAG parameters for perfect single crystal copper has been studied. At temperature close to the melting point, a double-dip in pressure-time profile is observed. It was shown that the first dip is due to loss of long range order and creation of stacking faults and not due to void formation.
4. Single crystals used in experiments have different types of defects (dislocations, impurities in parts per million, vacancies etc). Therefore NAG parameters have been obtained for single crystal copper with different defects (dislocations, vacancies etc).
5. For comparison with single crystal copper spallation experiments, a hierarchical multi-scale model is developed wherein the NAG parameters from the atomistic simulations are used in a macroscale hydrodynamic code. A good match for the spall strength has been obtained within an error of 20%.



To obtain the strength properties of single crystal copper, Split Hopkinson Pressure bar experiments at strain rates of 103/s have been carried out. The Johnson-Cook model parameters for material strength have been obtained. Neutron diffraction studies before and after impact show the broadening of the diffraction peaks which is the signature of increased density of defects.

A hierarchical multi-scale method to obtain fracture properties, given an inter-atomic potential, has been developed. The material strength which is an important input is obtained from experiment.

Publications

1. "Temperature sensitivity of void nucleation and growth parameters for single crystal copper: a molecular dynamics study", S. Rawat, M. Warriar, S. Chaturvedi and V. M. Chavan, *Modelling and Simulation in Material Science and Engineering* (19) (2011) 025007 (20 pp).
2. "Effect of material damage on the spallation threshold of single crystal copper: a molecular dynamics study", S. Rawat, M. Warriar, S. Chaturvedi and V. M. Chavan, *Modelling and Simulation in Material Science and Engineering* (20) (2012) 015012 (18 pp).
3. "Computation of spall data for single crystals with pre-existing defects using atomistic simulations", S. Rawat, V. R. Ikkurthi, M. Warriar, S. Chaturvedi, V. M. Chavan and R. J. Patel, Under review (*Acta Mechanica Sinica*).
4. "High strain rate deformation of single crystal copper: experiments and molecular dynamics simulations", S. Rawat et al, Under preparation.

Refereed Conferences:

1. "Effect of temperature on the void nucleation and growth parameters for single crystal copper", S. Rawat, M. Warriar, S. Chaturvedi and V. M. Chavan, *AIP Conf. Proc.* 1349 (2011) 87-88.
2. "Molecular dynamics simulations of crystal copper: Bulk modulus and shocks", M. Warriar, S. Rawat and S. Chaturvedi, *AIP Conf. Proc.* 1349 (2011) 95-96.
3. "Fracture during high velocity impact of copper plates: a molecular dynamics study", S. Rawat, M. Warriar, S. Chaturvedi and V. M. Chavan, *J. Phys.: Conf. Ser.* 377 (2012) 012104 (4pp).
4. "Excitation of characteristic modes of a crystal during solid fracture at high tensile pressure", S. Rawat, M. Warriar, D. Raju, S. Chaturvedi and V. M. Chavan, *J. Phys. Conf. Ser.* 377 (2012) 012107 (4pp).
5. "Reduction in spall threshold due to non-contact impact: a molecular dynamics study", S. Rawat, M. Warriar, S. Chaturvedi and V. M. Chavan, *AIP Conf. Proc.* 1447 (2012) 123-124.
6. "Activation of slip systems and shape changes during deformation of single crystal copper: a molecular dynamics study", S. Rawat, V. M. Chavan, M. Warriar, S. Chaturvedi, S. Sharma and R. J. Patel, *AIP Conf. Proc.* 1512 (2013) 84-85.
7. "Neutron diffraction measurements of dislocation density in copper crystals deformed at high strain rate", M. N. Rao, S. Rawat, S. Sharma, V. M. Chavan, R. J. Patel and S. L. Chaplot, *AIP Conf. Proc.* 1512 2013 526-527.
8. "Effect of strain rate on the void nucleation and growth characteristics in single crystal copper: a molecular dynamics study", S. Rawat, M. Warriar, S. Chaturvedi, V. M. Chavan and R. J. Patel, Accepted in 4th International Congress on Computational Mechanics and Simulation (ICCMS), IIT Hyderabad, India, December 9-12, 2012.'
9. "Multi-scale model for single crystal spallation at high strain rates", V. R. Ikkurthi, S. Rawat, R. Sugandhi, M. Warriar and S. Chaturvedi, Accepted in 4th International Congress on Computational Mechanics and Simulation (ICCMS), IIT Hyderabad, India, December 9-12, 2012.



Non-refereed Conferences:

1. "Molecular dynamics simulation studies of material failure under extreme conditions", S. Rawat, M. Warriar, S. Chaturvedi and V. M. Chavan, 54th DAE Solid State Physics Symposium (2009).
2. "Void nucleation and growth parameters for single crystal copper and their sensitivity to temperature", S. Rawat, M. Warriar, S. Chaturvedi and V. M. Chavan, First International Conference on Advances in Interaction and Multiscale Mechanics (AIMM10), May 31 - June 2, 2010, pp. 119, Jeju, Korea.
3. "Void nucleation threshold for single crystal copper and its validation by shock wave simulation", S. Rawat, M. Warriar, S. Chaturvedi and V. M. Chavan, Second International Conference on Advances in Nuclear Materials (ANM 2011), Feb 9 - 11, 2011, Mumbai, India.
4. "Multi-scale simulations of damage of perfect crystal copper at high strain rates", S. Rawat, M. Warriar, S. Chaturvedi and V. Ikkurthi, The ISAMP Topical Conference (TC 2012) "Laser interaction with atoms, molecules and clusters", Jan 9 - 12, 2011, Hyderabad, India.
5. "Computation of spall data for single crystals with pre-existing defects using atomistic simulations", S. Rawat, M. Warriar, S. Chaturvedi, V. M. Chavan and R. J. Patel, 9th International Conference on New Models and Hydrocodes for Shock Processes in Condensed Matter (NMH 2012), April 23 - 27, 2012, London, UK.

Work Presented:

1. "Computer simulations for high strain rate processes", V. R. Ikkurthi, S. Madhavan, A. Majalee, V. Mehra, V. Mishra, P. Pahari, S. Pahari, S. Rawat, N. Sakthivel, N. Shiv, C. D. Sijoy, M. Warriar and S. Chaturvedi, National Workshop on High Strain Rate Behaviour of Materials, Feb 25 - 26, 2010, Terminal Ballistics Research Laboratory, Ministry of Defence, Chandigarh, India.
2. "High velocity impact for determining materials properties under extreme conditions: simulations and experiment", S. Pahari, S. Madhavan, V. Mehra, C. D. Sijoy, S. Rawat, M. Warriar, I. V. V. Suryaprasad, N. Shiv and S. Chaturvedi, 25th National Symposium on Plasma Science and Technology, Dec 8-11, 2010, Institute of Advanced Study in Science and Technology, Guwahati, India.



Name : **Sibanarayan Tripathy**
Enrolment No. : CHEM01200704006
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Development of Asymmetric Routes to Biologically Active Cyclic Molecules: Synthesis of Carbocycles and Heterocycles

Abstract

The thesis is organized into 5 chapters which demonstrate a detailed work on asymmetric syntheses of cyclic molecules of biological relevance. In Chapter 1, a brief introduction of asymmetric synthesis of organic molecules has been provided. This chapter, also gave an elaborate description of various important parameters related to asymmetric synthesis viz substrate/reagent controlled reactions, different strategies of asymmetric transformation, different models associated with such reactions to obtain stereo-selectivity etc. In chapter 2, the importance and classification of the carbocyclic nucleosides based upon the ring size of the carbasugar has been explained in brief, followed by the endeavour on synthesis of the carbocycle core of 2', 3' – olefinic carbocyclic nucleoside Carbovir. Here a stereo-divergent route for the construction of the carbocyclic core of both (+)- and (-)-carbovir in their appropriate stereochemical form has been developed by the elegant utilization of the homoallylic alcohol obtained from easily accessible (*R*)-2,3-*O*-cyclohexylidene-glyceraldehyde of commercially available (*D*)-mannitol origin. The key step of the process involves the Luche's allylation of the synthesised allylic bromide with gaseous formaldehyde and RCM of a subsequent diene using Grubbs's first generation catalyst, which lead to the core cyclopentene unit. Synthesis of another homologue of the carbocyclic nucleoside Carbovir i.e. Homocarbovir, has been explained in the chapter 3 making use of the chiral template (*R*)-2,3-*O*-cyclohexylidene-glyceraldehyde in a different manner. The key steps in involves the stereoselective addition of the copper mediated vinyl magnesium bromide to an *E*- α,β -unsaturated ester followed by the RCM of the subsequent diene obtained in the process, which judicious exploitation of the chiral template (*R*)-2,3-*O*-cyclohexylidene-glyceraldehyde in a different manner to prepare several stereo-isomers of carbafuranose and their stereochemical assignment which have significant biological importance. The salient feature of this work was the construction of carbafuranose skeleton through intra-molecular allylation of an aldehyde intermediate. Chapter 5 describes the syntheses of some oxygenated heterocycles. The first part of the chapter describes a simple approach to produced two stereoisomers of 2,3,5-trisubstituted tetrahydrofurans in a single step through intra-molecular cyclisation during deketalisation of an intermediate, that was derived from the chiral template (*R*)-2,3-*O*-cyclohexylidene-glyceraldehyde. The moderate selectivity of this reaction and chromatographic separation of the diastereomers of the product proved beneficial to obtain two stereoisomers of the trisubstituted THF. However employing the same sequence of reaction starting from *syn*-homoallylic alcohol also produced trisubstituted tetrahydrofurans, but as a chromatographically inseparable mixture of diastereomers. The other part of this chapter dealt with an ongoing work on the synthesis of a macrolide, Decarestrictine-O, an inhibitor of cholesterol biosynthesis. Here the proposed plan was concerned with the construction of the required macrolide unit by RCM of a bisolefin intermediate. This is being obtained through the combination of two fragments of (*R*)-2,3-*O*-cyclohexylidene-glyceraldehyde and L-(+)-diethyl tartarate origin.



Publications

A. Published:

1. Chattopadhyay, A.; Tripathy, S. Stereodivergent route to the carbocyclic core of 2',3'-olefinic carbanucleosides: toward the synthesis of (L)-(+)- and (D)-(-)-carbovir. *J. Org. Chem.* **2011**, *76*, 5856–61.

B. Accepted:

1. Tripathy, S.; Chattopadhyay, A. (R)-2, 3-O-Cyclohexylidene-glyceraldehyde : a Useful Template for a Simple Entry into Carbafuranose Stereoisomers *Tetrahedron Asymmetry* **2012** (in press).

C. Manuscript under preparation.

1. Tripathy, S.; Chattopadhyay, A. A stereoselective route to carbocyclic core of 2',3'-olefinic carbanucleosides: towards the synthesis of homocarbovir.

D. Abstract presented in national conferences.

1. Tripathy, S.; Chattopadhyay, A. Synthesis of (L)-(+)- and (D)-(-)- Carbovir utilizing (R)-2, 3-cyclohexylidene-glyceraldehyde via RCM, Chemistry Research Scholar's Meet 2011, IGCAR, Kalpakkam, Chennai-India (oral presentation- 2011)
2. Tripathy, S.; Chattopadhyay, A. A Simple and Stereodivergent route towards the synthesis of (L)-(+)- and (D)-(-)- Carbovir, Research Scholar's Meet 2012,



Name : **R. Venkatesh**
Enrolment No. : MATH10201104007
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Unique Factorization of Tensor Products for Kac-Moody Algebras

Abstract

In the first part, we address a fundamental question, unique factorization of tensor products, that arises in representation theory. We consider integrable, category \mathcal{O} modules of indecomposable symmetrizable Kac-Moody algebras. We prove that unique factorization of tensor products of irreducible modules holds in this category, upto twisting by one dimensional modules. This generalizes a fundamental theorem of Rajan for finite dimensional simple Lie algebras over \mathbb{C} . Our proof is new even for the finite dimensional case, and uses an interplay of representation theory and combinatorics to analyze the Kac-Weyl character formula. In the second part, we get a new interpretation of the chromatic polynomials using Kac-Moody theory and derive some of its properties using this new interpretation.

Publications

1. R. Venkatesh, Sankaran Viswanath. Unique factorization of tensor products for Kac-Moody algebras. *Advances in Mathematics*, 231(6):3162-3171, 2012.



Name : **Girish Kumar Padhy**
Enrolment No. : CHEM02200704016
Constituent Institute : Indira Gandhi Centre for Atomic Research, Chennai
Title : Study of Diffusible Hydrogen in Steel Welds Using indigenously Developed Hot-Extraction Techniques

Abstract

In this study, two hot extraction techniques were developed for diffusible hydrogen (H_D) measurement in steel welds. One is based on a proton exchange membrane based hydrogen sensor (PEMHS) and the other based on Gas Chromatograph (GC). Using the new techniques, diffusible hydrogen was collected from weld specimens at higher temperatures (400°C) and the results obtained were compared with those obtained from standard mercury method for H_D measurement recommended by ISO 3690. One to one correlation is obtained between the results for different welding consumables of varying diffusible hydrogen content. Further, employing the PEMHS technique, a systematic investigation was carried out to study the effects of preheat and post-heating on the H_D contents of welds. This study has confirmed that preheating combined with post-heating even at lower temperatures is better in reducing diffusible hydrogen than preheating alone at higher temperature. This study has also confirmed that, the best way to measure H_D content in preheated weld specimens is by removing the specimens from the welding fixture for a condition in which specimen is cooled down to 100°C . Though preheating and post heating are widely used to remove hydrogen from welds, no systematic study on quantitative estimation of hydrogen remaining in welds after preheating and post heating is reported so far. These new techniques were also used to estimate apparent diffusivity of hydrogen in steels at different temperatures. For this study, cylindrical specimens of mild steel, 2.25Cr-1Mo steel and modified 9Cr-1Mo steel were electrochemically charged with hydrogen. Hydrogen evolved from steel specimens for different time durations at 25, 100, 200, 300 and 400°C was measured. The hydrogen evolution data were used in the diffusion equation of cylinder to determine the apparent diffusivity of hydrogen in these steels. For more accurate determination of apparent diffusivity, a numerical method was proposed in which hydrogen lost before the start of the measurement and the corresponding time lags involved in the hydrogen loss were calculated. These data were used to correct the original hydrogen evolution data obtained using the new hot extraction methods. From the corrected hydrogen evolution data, the apparent diffusivity of hydrogen in these steels was determined. The results obtained in this study agreed well with those reported in the literature. The apparent diffusivity of hydrogen in steel was found to be decreasing with increase in the alloy content of steel. This also explained why 9Cr-1Mo has higher susceptibility for hydrogen cracking than mild steel even though it has lower H_D content.

Publications

I. Publications in Refereed Journals

1. G. K. Padhy, V. Ramasubbu, N. Murugesan, C. Ramesh and S.K. Albert: Developing a sensor for diffusible hydrogen measurement, *Welding Journal*, 2011, Vol. 90, No. 3, 47-53.
2. G. K. Padhy, V. Ramasubbu, N. Murugesan, C. Ramesh and S.K. Albert: Hot extraction of diffusible hydrogen and its measurement using a hydrogen sensor, *Welding In the World*, 2012, Vol. 56, No. 7/8, 18-25
3. G. K. Padhy, V. Ramasubbu, N. Murugesan, C. Ramesh and S.K. Albert: Effect of preheat and post heating on the diffusible hydrogen content of welds, *Science and Technology of Welding and Joining*, 2012, Vol. 17, No 5, 408-413



4. G. K. Padhy, V. Ramasubbu, N. Murugesan, C. Ramesh and S.K. Albert : Diffusible hydrogen measurement in steel welds using an electrochemical hydrogen sensor, *Indian Welding Journal*, 2012, Vol.45, No.1, 35-46
5. G. K. Padhy, V. Ramasubbu, N. Murugesan, N. Parvathabarthini, C. Ramesh and S.K. Albert: Determination of apparent diffusivity of hydrogen in 9Cr-1MoVNbN steel using a hot extraction technique, *International Journal of Hydrogen Energy*, 2013, Vol. 38, 10683-10693

II. Publications under progress

1. G. K. Padhy, V. Ramasubbu, N. Parvathabarthini, and S.K. Albert: Effect of composition/alloying elements on the apparent diffusivity of hydrogen in steel (*Manuscript submitted to Metallurgical and Materials Transactions A*)
2. G. K. Padhy, V. Ramasubbu, and S.K. Albert: Rapid determination of diffusible hydrogen in steel welds using a modified gas chromatography facility (*Manuscript submitted to Journal of Testing and Evaluation*)

III. Papers presented in Conferences and Assemblies

1. G. K. Padhy, V. Ramasubbu, N. Murugesan, C. Ramesh and S.K. Albert: Diffusible hydrogen measurement in welding consumables using a new proton-exchange-membrane based hydrogen sensor, *National Welding Seminar*, 4th-6th February, 2009, Mumbai, India.
2. G. K. Padhy, V. Ramasubbu, N. Murugesan, C. Ramesh and S.K. Albert: : Diffusible hydrogen measurement in steel welds using an electrochemical hydrogen sensor, *National Welding Seminar*, 21st-23rd December, 2010, Visakhapatnam, India.
3. G. K. Padhy, V. Ramasubbu, N. Murugesan, C. Ramesh and S.K. Albert: Hot extraction of diffusible hydrogen and its measurement using a hydrogen sensor, *64th Annual Assembly and International Conference of International Institute of Welding*, 17th-22nd July, 2011, Chennai, India.
4. G. K. Padhy, V. Ramasubbu, K. R. Rangarajan, M. K. Singari, S. K. Albert: A new gas chromatography facility for rapid determination of diffusible hydrogen in steel welds. Paper ID: 263, *National Welding Seminar*, 7-9th February, 2013, Bangalore, India
5. S. K. Albert, G. K. Padhy: Measurement of diffusible hydrogen and hydrogen diffusivity using a newly developed hydrogen sensor. Paper ID: 512, *National Welding Seminar*, 7-9th February, 2013, Bangalore, India

IV. Award

1. ESAB India Award for Best Paper among All Categories: Diffusible hydrogen measurement in steel welds using an electrochemical hydrogen sensor, G. K. Padhy, V. Ramasubbu, N. Murugesan, C. Ramesh and S.K. Albert, *National Welding Seminar*, 21st-23rd December, 2010, Visakhapatnam, India.



Name : **Kalpataru Panda**
Enrolment No. : PHYS02200704023
Constituent Institute : Indira Gandhi Centre for Atomic Research, Chennai
Title : Scanning Tunneling Microscopy Studies on Enhanced Electron Field Emission Properties of Modified Nanostructured Diamond Films

Abstract

Diamond and related materials have enormous potential applications due to their interesting physical and chemical properties. Depending on the diamond particle size, diamond films are classified into microcrystalline (MCD), nanocrystalline (NCD) and ultrananocrystalline (UNCD). Diamond films are used as excellent electron field emitter devices due to their low work function and negative electron affinity properties. In this thesis, systematic studies has been made to improve and understand the mechanism of electron field emission (EFE) properties by (i) N^+ ion implantation to UNCD films (ii) N^+ ion implantation to UNCD films (ii) N^+ ion implantation to hybrid structured diamond films, where a UNCD layer is used as a interlayer for the growth of MCD film (MCD/UNCD), and by (iii) depositing a thin layer of iron (Fe) on MCD and UNCD films followed by post-annealing in H_2 atmosphere. N^+ ion implantation/post-annealing is seen to significantly enhance the EFE properties of UNCD an hybrid structured MCD/UNCD films. In order to investigate the mechanism of enhanced EFE properties, Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM) and scanning tunneling spectroscopy (STS) studies were carried out on the implanted and un-implanted films. XPS measurements shows increased sp^2 phase content and C-N bonding fraction in N^+ ion implanted and post-annealed films. Transmission electron microscopic analysis revealed that the mechanism behind the enhanced EFE properties in N^+ ion implanted/post-annealed films is due to the defects in the diamond grains and the formation of nanographitic phase surrounding the diamond grains. Current imaging tunneling spectroscopy (CITS) in scanning tunneling spectroscopy (STS) mode clearly shows increased density of emission sites in N^+ implanted/post-annealed UNCD and MCD/UNCD films as compared to their corresponding as-prepared ones. Hence, the amount of nano graphitic phase is found to be crucial for enhancing the EFE properties. Further, to increase the nanographitic phase content, Fe is used as a catalyst. Fe is used as a catalyst. For this, a thin layer of Fe film is coated on MCD and UNCD films followed by post-annealing in H_2 atmosphere which produces nanoparticles of Fe and Fe_3C . The EFE properties of Fe-coated/post-annealed MCD and UNCD films are found to be better and further the EFE properties of Fe coated UNCD films are better than that of Fe coated MCD films. The mechanism behind the enhanced EFE properties of Fe-coated/post-annealed UNCD films are explained by the microstructural investigation which shows the formation of high volume fraction of nanographitic phase surrounding the Fe (or Fe_3C) nanoparticles.

Publications

Publications in Journals

1. Direct observation of enhanced emission sites in nitrogen implanted hybrid structured ultrananocrystalline diamond films. Kalpataru Panda, Huang-Chin Chen, B. Sundaravel, B.K Panigrahi, I-Nan Lin, J. Appl. Phys. 113, 054311 (2013).



2. The induction of nanographitic phase on Fe coated diamond films for the enhancement in electron field emission properties. Kalpataru Panda, B.Sundaravel, B.K. Panigrahi, H-C Chen, P-C Huang, W-C Shih, S-C Lo, L-J Lin, C-Y Lee, I-Nan Lin, J. Appl. Phys. 113, 094305 (2013).
3. Tribological properties of N⁺ ion implanted ultrananocrystalline diamond films. Kalpataru Panda, N. Kumar, B. K. Panigrahi, S. R. Polaki, S. Dhara, B. Sundaravel, S. Dash, A. K. Tyagi, I-Nan Lin, Tribol. Inter. 57, 124 (2013).
4. Direct observation and mechanism of increased emission sites in Fe-coated microcrystalline diamond films. Kalpataru Panda, B. Sundaravel, B. K. Panigrahi, P-C Huang, W-C Shih, H-C Chen, I-N. Lin, J. Appl. Phys. 111, 124309 (2012).
5. N-ion implantation of micro/nanocrystalline duplex structured diamond films for enhancing their electron field emission properties. Kalpataru Panda, B. Sundaravel, H-F Cheng, C-C Horng, H-Y Chiang, H-C Chen, I.-N Lin, Surf. Coat. Tech, DOI:10.1016/j.surfcoat.2012.05.107.
6. Structural and electronic properties of nitrogen ion implanted ultrananocrystalline diamond surfaces. Kalpataru Panda, B. Sundaravel, B. K. Panigrahi, P. Magudapathy, D.N. Krishna, K.G.M. Nair, H-C Chen, I-Nan Lin, J. Appl. Phys. 110, 044304 (2011).

Conferences

1. Enhanced field emission and scanning tunneling microscopy studies of iron coated microcrystalline diamond films Kalpataru panda, B. Sundaravel, B.K. Panigrahi, K.G.M Nair, I-Nan Lin ICONSAT, Hyderabad, 2012, India.
2. Electronic and field emission properties of ultrananocrystalline diamond surfaces Kalpataru Panda, B. Sundaravel, B. K. Panigrahi, K. G. M. Nair, I-Nan Lin, International Conference on Carbon Nanotechnology, IIT Kanpur, 2010, India.



Name : **S. Sheerazuddin**
Enrolment No. : MATH10200604022
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Temporal Specifications of Client-Server Systems and Unbounded Agents

Abstract

We study the formal specification and verification of two kinds of client-server systems in this PhD thesis: Single Client Multiple Server (SCMS) Systems and Single Server Multiple Client (SSMC) Systems.

In SCMS systems, a single client interacts with a host of servers to obtain some service where the number of servers is fixed a priori. We propose a local temporal logic called w-LTL with a novel concurrent present modality, called now, to describe valid patterns of interactions of SCMS systems and show that the satisfiability and model checking problems are decidable.

In SSMC systems, an unbounded number of clients of different types need the service of a single server where the number of client types is fixed beforehand. In the literature, SSMC systems appear in two flavours: discrete and session-oriented. For each paradigm, we present an automaton model, System of Passive Clients (SPS) for discrete services and System of Active Clients (SAS), for session-oriented services. We show that SAS are equivalent to multi-counter automata, whereas SPS is a subclass of SAS.

The logical language to specify and verify SPS-like systems, called LSPS, consists of MFO sentences closed over temporal modalities. We show the satisfiability and model checking of LSPS to be decidable using a formula automaton construction.

We propose a fragment of monadic monodic temporal logic as the specification language for SAS. We present a formula automaton construction, using a multi-counter automaton, that leads to a non-elementary decision procedure for the satisfiability of LSAS.

Publications

1. S. Sheerazuddin, "Automata Models for Services with Unboundedly Many Clients", In International Conference on Software and Computing Technology (ICSCT), 2010.
2. S. Sheerazuddin, "Temporal Specifications for Services with Unboundedly Many Passive Clients", In International Conference on Distributed Computing and Networking, (ICDCN) 2011.
3. R. Ramanujam and S. Sheerazuddin, "Temporal Specifications for Services with Unboundedly Many Active Clients", In International Conference on Distributed Computing and Internet Technology (ICDCIT), 2011.



Name : **Manoj Kumar Singh**
Enrolment No. : PHYS03200704008
Constituent Institute : Raja Ramanna Centre for Advanced Technology, Indore
Title : Computational Study of Growth Morphology of Molecular Crystals

Abstract

In this thesis, many aspects of prediction of crystal morphology have been studied. Most important of all, is the role of molecular orientation and growth environments including the nature of solvent in determining the crystal shape. The purpose of these investigations is to obtain a comprehensive understanding of the crystal growth and in particular the role played by the solvent, external growth factors and additives can have on the growth process and the resulting growth morphology. An additive in this context does not mean solute added to the solution, but can also be the solvent itself since it is well known that the solution from which a crystal is grown can change the habit dramatically. Understanding the molecular mechanisms of crystal growth and precise control of the growth environments are essential steps towards controlling the crystal growth, morphology and shape and to study polymorphism and nucleation, which are of prime interest and importance in chemical and pharmaceutical industries. Since crystals interact with their surrounding predominantly through their surfaces, the shape of a crystal influences their chemical and physical properties. This thesis provides a systematic method for studying and incorporating the effects of molecular orientations of growth units, solvents and growth environments on crystal morphology of molecular crystals.

The calculations of structure and lattice energies of different molecular crystals have been discussed in Chapter 2. A growth model is proposed in Chapter 3, which considers the effects of molecular orientation on crystal morphology. It is based on the assumption that growth units directly incorporated into the crystals through their surfaces rather than the attachment of 2-D slices of thickness of one interplanar layer. It clearly shows that the role of molecular orientations and surface relaxation need to be considered to predict crystal morphology from vapour phase. The "riddle" of the unidirectional growth and dissolution of opposite and hemihedral faces of two polar crystals namely α -resorcinol and urea crystals from vapour phase are described in Chapter 4. It has been shown that the root cause of the asymmetric growth and dissolution of (011) and (111) faces of α -resorcinol and urea crystals, respectively, are intrinsic properties of polar crystals on which surface relaxation and solvent further enhances the asymmetry which is in agreement with the experimental observations.

The solvent-induced habit modification of different crystals is studied in Chapter 5. In this chapter, a computational crystal growth model is described to investigate the mechanism through which solvent interacts with the crystal surfaces. The effects of many external growth factors like level of supersaturation, temperature and solubility on crystal morphology are investigated in this chapter. Emphasis is placed on the accurate representation of interfacial structure, adsorption energies of the solute-surface and solvent-surface. Based on the analysis of interfacial structure and growth environment, the expressions for growth and dissolution rates have been derived and presented in Chapter 5. It relates level of supersaturation, temperature, solubility, bonding energies of solute-crystal, solvent-crystal to the rate of growth/dissolution. The method is applied to urea and β -succinic acid crystals to calculate growth rate of different faces and growth shapes as functions of supersaturation and temperature from vapor and different solvents. The predicted crystal



morphology as function of supersaturation and temperature are in agreement with the corresponding experimental observations. Unidirectional growth and dissolution at the opposite and hemihedral faces of α -resorcinol and (R, S) alanine crystals from aqueous solution are also investigated using the discussed method. In case of growth and dissolution of (011) and (0-resorcinol and (R, S) alanine crystals from aqueous solution are also investigated using the discussed method. In case of growth and dissolution of (011) and (0 1 1) faces of α -resorcinol crystal, we find that former face has higher affinity with water than the latter.

Publications

A. International Journals:

1. "Asymmetrical Growth and Dissolution along Polar Axis of α -Resorcinol Crystal: Role of Solvent and External Environment" M. K. Singh and Arup Banerjee, *CrystEngComm*, 2013, DOI:10.1039/C3CE41155A (in press).
2. "Role of solvent and external environments to determine growth morphology of molecular crystals" M. K. Singh and Arup Banerjee, *Crystal Growth & Design*, 2013, 13, 2413-2425.
3. "Growth and dissolution mechanism at the opposite and hemihedral faces of polar crystals" M. K. Singh and Arup Banerjee, *CrystEngComm*, 2013, 15, 4143-4152.
4. "Role of molecular orientation and surface relaxation on vapor growth shape of molecular crystals" M. K. Singh and Arup Banerjee and P. K. Gupta, *Crystal Growth Design*, 2012, 12, 732-741.
5. "Simulating vapour growth morphology of crystalline urea using modified attachment energy model" M. K. Singh and Arup Banerjee and P. K. Gupta, *J. Crystal Growth*, 2012, 343, 77-85.
6. "Atomic-scale study of vapour growth morphology of crystalline urea" M. K. Singh and Arup Banerjee, *Cryst. Res. Tech.* 2011, 46, 1035-1043.

Under preparation:

1. "Predicting polar morphology of urea crystal from vapour phase" M. K. Singh *et al.*
2. "Role of Dispersive Interactions in Predicting Lattice Energy and Structure of Organic Crystals by First-Principles Method" M. K. Singh *et al.*

B. International/National Conferences

1. "Ab initio investigation of structure and lattice energy of molecular crystals" M. K. Singh and Arup Banerjee, National Laser Symposium, Crystal Growth Centre, Anna University, Chennai, Jan 9-12, 2012.
2. "Uncovering the mode of action of solvent on molecular crystal growth" M.K. Singh and Arup Banerjee, Proceedings of the National Symposium on Growth of Detector- Grade Single Crystals-2009, November 19-21, 2009.
3. "Atomic scale investigations of vapour growth morphology of urea crystal" M.K. Singh and Arup Banerjee, 16th International Conference on Crystal Growth in Beijing, China from 8 -13 August 2010.



Name : **Amitkumar Gaibidas Fulzele**
Enrolment No. : LIFE09200604006
Constituent Institute : Tata Memorial Centre, Parel, Mumbai
Title : Keratin Profile in Oral Cancer

Abstract

Keratins play a major role in several cellular functions. Each tissue expresses a specific set of keratins. The immense potential of keratins as diagnostic and prognostic markers for different cancers is emerging. Oral cancer is the fifteenth most common cancer worldwide. However, comprehensive information on the profile of keratins using antibodies which are not well characterized and exhibit cross reactivity to this set of very homologous proteins. A few recent proteomic studies have reported the identification of keratins in head and neck cancer. Majority of the studies have used tissues from the head and neck region without specifying subsites which are reported to have unique molecular characteristics. To obtain a comprehensive profile of the keratins enriched preparations of keratins from cancer of the gingivo buccal complex (GBC), a subsite of the oral cavity, were analysed using mass spectrometry two dimensional gel electrophoresis, (2DE), Western blotting, silver staining of 2DE gels and immunohistochemistry. The study revealed the presence of K1, K2, K5, K6A, K6B, K6C, and K10 in normal and tumor tissues to nearly the same extent by mass spectrometry. Results clearly showed the absence of K4 and K13 and presence of K14, K16, and K17, in cancers of the GBC and combination of these expression patterns in the surgical cut margins. Further this thesis reports that K13 is glycosylated in normal tissues from the GBC. Several studies have reported the aberrant expression of Keratin 18 in oral cancer. K 18 was seen with an antibody to K 18 (clone CY 90). In depth analysis revealed that the antibody to K 18 cross reacted with K 13 and actin. Thus this study emphasizes the necessity of mass spectrometry for validation of antibody based findings and caution in interpretation when dealing with very homologous proteins. In summary, this well characterized profile of keratins has potential to be used in the clinics.

Publications

Published:

1. Fulzele A, Malgundkar S, Govekar R, D'cruz A, Chaturvedi P, Patil A, Kane S, Zingde SM.: Keratins in oral cancer: Necessity of mass spectrometry for validation of antibody based identifications. J. Proteomics. 2012, 75, 8, 2404-2416.

Communicated: Manuscript ready and to be submitted shortly.

1. Amit Fulzele, Siddhi A. Malgundkar, Rukmini B. Govekar, Asawari Patil, Shubhada V. Kane, Pankaj Chaturvedi, Anil K. D'Cruz, and Surekha M. Zingde: Proteomic profile of keratins in cancer of gingivo buccal complex: Consolidating insights for clinical applications. Target Journal: Journal of Pathology



Name : **Gaurav Kumar**
Enrolment No. : LIFE09200704008
Constituent Institute : Tata Memorial Centre, Parel, Mumbai
Title : Effect of Curcumin and Black Tea Polyphenols on Carcinogen-Induced Cell Proliferation and Apoptosis in Experimental Models

Abstract

Plant-derived natural compounds are receiving increasing attention as chemopreventives because of their low toxicity and high tolerability. The efficacy of polyphenols has been established when administered before or after the carcinogen treatment and have been shown to modulate carcinogen-induced incidence/multiplicity/latency period of tumor development.

In the first objective, we have examined the anti-promoting mechanisms of polymeric black tea polyphenols (PBPs). Pre-treatment with PBP 1-3 fractions were more effective than PBP-4 & -5 in decreasing the TPA-induced translocation of protein kinase C (PKC) from cytosol to membrane whereas levels of PKCs δ and ξ in cytosol/membrane were similar in all the treatment groups. Both PBP-3 and PBP-5 were observed to decrease the PKC phosphorylation and upstream kinase phosphorylation / activity of PI3K and AKT1. Altogether, PBP-mediated decrease in TPA-induced PKC phosphorylation correlated well with decreased TPA-induced NF- κ B phosphorylation and down-stream target proteins associated with proliferation, apoptosis, and inflammation in mouse skin.

In the second objective, we have evaluated the post-treatment effects of dietary turmeric on markers related to apoptosis, cell proliferation, and inflammation in 7,12-dimethylbenz(a)anthracene (DMBA)-induced hamster buccal pouch (HBP) tumors. Result suggests that decrease in tumor growth was due to the modulation of cellular pathways associated with cell proliferation and apoptosis. Some of these proliferation and apoptosis-related markers are likely to be helpful in monitoring clinical trials and evaluating drug effects.

In the third objective, post-treatment effects of dietary curcumin on the levels of benzo(a)pyrene [B(a)P]-induced DNA adducts in mouse tissues were investigated. Quantitative comparisons suggested time dependent decrease in the levels of adducts in B(a)P-treated animals and the observed decrease was further enhanced by curcumin exposure when compared to the levels in time-matched controls. Results suggested enhancement of B(a)P-induced apoptosis in liver and lungs by curcumin during 24-120 h while there was no such enhancement observed at 8-28 days. Results suggest curcumin-mediated enhancement in apoptosis and DNA repair during 24-120 h and adduct dilution and/or DNA repair during 8-28 days to be the reason for the observed higher decrease of BPDE-DNA adducts.

Chemopreventive efficacy of PBPs or turmeric/curcumin during different stages of carcinogen-induced tumorigenicity has been demonstrated in several experimental models. The mechanisms implicated in the inhibition of carcinogenesis by BTPs involve modulation of signalling kinases or xenobiotic-induced activation/ translocation of kinases or modulation of tumor-induced responses ultimately leading to effects on multiple signaling pathways and genes. Considering the reported biological effects of both PBPs or turmeric/curcumin *in vivo* and the potential for the development of modern medicine, further investigations in well-designed experimental and human intervention studies are needed. On-going studies are likely to help in determining the usefulness of curcumin in prevention and therapy of specific diseases including cancer.



Publications

- 1) Gaurav Kumar, Prerana Dange, Vaishali Kailaje, Milind M. Vaidya, Asha g. Ramchandani, Girish B. Maru . Polymeric black tea polyphenols modulate the Localization and activity of 12-O-tetradecanoyl phorbol- 13-acetate-mediated kinases In mouse skin: mechanisms of their anti-promoting action. *Free Radical Biology & Medicine*, 2012,53: 1358-1370.
- 2) Gaurav Kumar, Pooja Tejpara, Girish B. Maru. Dietary turmeric post-treatment decreases DMBA-induced hamster buccal pouch tumor growth by altering cell Proliferation and apoptosis related markers. *Journal of environmental Pathology, Toxicology , and Oncology*, 2012, 31(4): 295-312.
- 3) Gaurav Kumar, Shubhangi P. Pillare and Girish B. Maru. Black tea polyphenols mediated *in vivo* cellular responses during carcinogenesis. *Mini- Reviews in Medicinal Chemistry*, 2010, 10: 492-505.
- 4) Girish B. Maru , Asha G. Ramchandani, Gaurav Kumar, Rachana Garg. Curcumin-mediated cellular responses in chemical carcinogenesis: *In vivo* Studies. Chapter Xth, 181-204, 2010. *Bioactive foods and Extracts Cancer treatment and Prevention*. Edited By Ronald Ross Watson and Victor T. Preedy.



Name : **Atul Pranay**
Enrolment No. : LIFE09200604004
Constituent Institute : Tata Memorial Centre, Parel, Mumbai
Title : Profiling of Autoantibodies to Tumor Antigens from Cancer of the Gingivo-Buccal Complex using Immunoproteomics

Abstract

Head and Neck cancer is a major cancer in India and cancer of the oral cavity is seen in ~25% of the patients reporting at the hospital. Of these majority are afflicted with cancer of the gingivo-buccal complex, a subsite of the oral cavity, due to the habit of chewing tobacco. Biomarkers are required to complement clinic-pathological findings for a more accurate prediction of individual patient's prognosis and determining effective therapy. Immunoproteomics is being used as an important tool to assess autoantibodies as biomarkers to tumor associated antigens, since it involves use of blood which can be obtained by less invasive techniques. Earlier investigations in the laboratory had identified twelve antigens which elicit an autoantibody response using immunoproteomics approach. The autoantibody response was higher in individuals with cancer.

This thesis investigates the utility of these tumor associated antigens in a new set of samples using immunoproteomics for their potential for early detection and prognosis for cancer of the gingivobuccal cancer. Data emerging from immunoproteomics evaluation using serum from individuals with and without tobacco habits, individuals with an early lesion ie leukoplakia and those with cancer of the gingivobuccal complex with T1/T2 and T3/T4 tumors shows that autoantibody response to antigens increases from those individuals without tobacco habits to those with lesions and cancer with increasing tumor size, supporting that the autoantibody response *could be harnessed for early detection*. This is further strengthened in a combined analysis done by pooling immunoproteomics data reported earlier from the laboratory.

Evaluation of *prognostic utility* shows that the autoantibody response against α ENO and HSP70 provides an additional parameter for predicting disease free survival and recurrence and may be utilized along with nodal involvement and differentiation status for better prognosis of cancer of GBC. In a multivariate analysis the relative risk of recurrence is 3.41 for patients who exhibit autoantibody response to both the antigens.

To *prepare a platform* such as a protein array or ELISA for assessment of antibody response, recombinant proteins of the antigens were cloned and purified. These were arrayed on a dot blot, used for ELISA and multiwesterns and autoantibody response was determined. The data emerging from each method were compared and the pros and cons of each platform assessed in the light of the differences in the technologies and the data obtained vis a vis the 2DE immunoproteomics approach. Results indicate that epitope presentation and post translational modifications may be important parameters for autoantibody evaluation when different techniques are used. These could be some of the reasons why several of the biomarkers do not reach the clinics as they cannot be validated by different technologies and attention to these parameters is necessary while generating multiplex arrays for validation of data in large sample sizes for translation into the clinics.

The thesis work has resulted in a Publication: Pranay et al. Proteomics Clin. Applications. Special issue; Focus on Cancer Proteomics, 7, 392-402, 2013



Publications

Published

1. Sanjeev Shukla, Atul Pranay, Anil K. D'Cruz, Pankaj Chaturvedi, Shubhada V. Kane, Surekha M. Zingde. Immunoproteomics reveals that cancer of the tongue and the gingivo-buccal complex exhibit differential autoantibody response. *Cancer Biomarkers*, 5, 127-135, 2009.
2. Pranay A, Shukla S, Kannan S, Malgundkar SA, Govekar RB, Patil A, Kane SV, Chaturvedi P, D'Cruz AK, Zingde SM. Prognostic utility of autoantibodies to α -enolase and HSP70 for cancer of the gingivo-buccal complex using immunoproteomics. *Proteomics Clin Appl*. 2012 Nov 17. doi: .1002/prca.201200081. [Epub ahead of print] PMID:23161576



Name : **Subhra Rani Patra**
Enrolment No. : ENGG02200704007
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Development of Computational Intelligence Systems for
Parameter Estimation and Event Identification in Fast Breeder
Reactors

Abstract

Computational intelligence is an area of applied research involving the study of adaptive mechanisms to enable or facilitate intelligent behavior in complex and changing environments. A computationally intelligent system deals with numerical (low-level) data, has pattern recognition component and it begins to exhibit computational adaptability, computational fault tolerance and speed approaching human-like turnaround, error rates that approximates human performance. The main building blocks of computational intelligence are artificial neural network, fuzzy logic, evolutionary computing, genetic algorithm and artificial life.

Modern nuclear power plant is a very complex arrangement of machinery consisting of huge number of control and support systems. Implementation of computational intelligence in the nuclear reactor domain is a challenging task due to its stringent safety regulations, but is extremely promising in solving many intricate problems pertaining to nuclear environment. In real time it is possible to implement intelligent systems in the form of neural network, data mining, expert system etc. for modeling the nuclear power plant. Neural network modeling is one among the data driven technique which is a powerful tool for identification of relevant physical parameters and is more advantageous compared to the traditional methods of plant diagnostics. A system can be modeled using neural network without having much knowledge of its internals.

In this thesis neural network based algorithms have been implemented for parameter estimation and event identification in fast reactors. The algorithms employed are: standard back propagation algorithm, radial basis function algorithm and variants of standard back propagation algorithms and the results are compared for all the case studies. A neural network based genetic algorithm has also been implemented for parameter estimation of Fast Breeder Test Reactor and the results are compared with neural network based standard back propagation algorithm.

This thesis summarizes the comprehensive study of implementation of computational intelligence systems in nuclear reactors as intelligent monitors. It provides the detailed description of the implementation of computationally intelligent models for parameter estimation in intermediate heat exchanger of Fast Breeder Test Reactor (FBTR) and neutronics system of Prototype Fast Breeder Reactor (PFBR). The parameters estimated are: sodium temperature in intermediate heat exchanger of FBTR and reactor power in PFBR. It briefly covers the event identification in neutronics system and primary sodium circuit system of PFBR. The events detected are: control and safety rod withdrawal event in neutronics system and primary sodium pump trip, primary sodium pump seizure and primary pipe rupture of primary sodium circuit of PFBR.

A neural network model has been proposed to estimate the value of temperature parameters in fast breeder reactor subsystems. Supervised back propagation algorithm has been employed and fine-tuned for this purpose. From the results obtained, it is shown that this algorithm shows faster convergence and takes less computation time compared to models developed based on physical relations.



A comparison study of back propagation and radial basis function algorithm is carried out for process modeling of temperature parameters of intermediate heat exchanger of FBTR. From the results, radial basis function algorithm is found to have faster convergence with less number of iterations. Reactor power estimation is also carried out implementing back propagation algorithm to multi layer perceptron model.

Neural network model has been implemented for identification of events or unsought occurrence of plant conditions which affect the safe operation of plant. The neutronics system and primary sodium circuit related events of PFBR have been detected using neural network algorithms. The event related input data has been generated from in-house developed thermal hydraulics code and has been validated as per the event analysis reports of PFBR. Four different events are taken together in a single neural network and back propagation algorithms and its variants are implemented. From the results it is observed that the neural network could be able to identify the events successfully. A hybrid genetic algorithm based neural network model has been employed for parameter estimation of intermediate heat exchanger of FBTR and the results are compared with standard back propagation algorithm. From the achieved results, it could be observed that genetic algorithm based neural network has faster convergence with less computation time in comparison with artificial neural network based standard back propagation algorithm. The experimental results obtained in this thesis show that artificial neural network could be used to estimate the parameters and detect the events of subsystems accurately and consistently, which will be an aid to operators handling non-linear complex systems in nuclear reactors.

Publications

1. Subhra Rani Patra*, R. Jehadeesan, S. Rajeswari, S.A.V Satya Murty, Artificial Neural Network model for IHX of Nuclear Reactor, *International Journal of Computer Applications*, 1 2010 65-72
2. Subhra Rani Patra*, R. Jehadeesan, S. Rajeswari, Indranil Banerjee, S.A.V Satya Murty, G. Padmakumar, M. Sai Baba, Neural Network modeling for evaluating Sodium temperature of Intermediate Heat Exchanger of Fast Breeder Reactor, *Advances in Computing*, 2 2012 16-22
3. Subhra Rani Patra*, R. Jehadeesan, H. Seetha, T. Jayanthi, S. Rajeswari, S.A.V Satya Murty, M. Sai Baba, Event Identification in Prototype Fast Breeder Reactor Subsystem Using Artificial Neural Network, *International Journal of Applied Information System*, 4 2012 1-9
4. Subhra Rani Patra*, R. Jehadeesan, S. Rajeswari, S.A.V. Satya Murty, M. Sai Baba, Development of Genetic Algorithm based Artificial Neural Network for Parameter Estimation of Fast Breeder Reactor Subsystem, *International Journal of Soft Computing and Engineering* 2 2012 87-90



Name : **Satinath Ghosh**
Enrolment No. : CHEM01200604014
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Theory and Modelling of Nucleation and Interfacial Phenomena

Abstract

The thesis is organized into seven chapters which demonstrate the theoretical investigations of different modes of vapour to liquid nucleation phenomena and also the interfacial properties of spherical and planar vapour-liquid interface. A realistic density profile i.e. an exponential density profile at vapour-liquid interface and a suitable local Helmholtz free energy density have been modelled to achieve a simple and analytical solution to these problems. In Chapter 1, a brief introduction to the general nucleation and interfacial phenomena has been provided which includes the historical back ground of classical nucleation theory (CNT), current trends in the theory of vapour to liquid nucleation, kinetic theory of nucleation, over view of the theory of vapour-liquid interface, over view of the density functional theory (DFT) and a brief description of nucleation experiments etc. In chapter 2, CNT, a DFT based formalism and a modified version of CNT for homogeneous nucleation have been discussed. The calculation of the density profile of nucleated droplet, critical size, nucleation barrier and free energy of formation of droplet as a function of supersaturation are the outcome of this chapter. Apart from homogeneous nucleation, the effect of the heterogeneity i.e. the droplet formation on the planar surface of a solid substrate and also on the spherical surface (seed mediated nucleation) have been investigated by applying both CNT and DFT and presented in chapter 2 and chapter 3 respectively. The effect of solid-fluid interaction energy, size of the seed etc. on the various properties such as formation free energy, nucleation barrier and shape of the droplet etc have been described. A shape wise mechanistic pathway during the course of nucleation on spherical seed has been demonstrated here. The work on seed mediated vapor to liquid nucleation is a general one where the results of homogeneous nucleation have been obtained at one end of the seed size (i.e. zero size of seed) whereas the heterogeneous nucleation on the flat surface is obtained on the other side (when the radius of the seed is infinity). A DFT formalism for the calculation of various interfacial properties including surface tension, density profile, thickness of the vapor-liquid planar interface have been discussed in chapter 5. A new scheme of calculating the surface tension of real fluids such water, heavy water etc over a wide range of temperature from triple point to critical point quite accurately has been shown in chapter 5. In chapter 6, a DFT based methodology for the calculation of size dependent interfacial properties have been demonstrated. The surface tension, density profile, temperature-density diagram, width of the interface etc. of liquid droplet-vapor interface and also for bulk liquid-vapor interface have been compared in this chapter. The numerical solution with the exact density also supports the modeling of the present density profile. The overall achievements of the present thesis have been briefly concluded in chapter 7.

Publications

1. Homogeneous nucleation in vapor-liquid phase transition of Lennard-Jones fluids: A density functional theory approach. Satinath Ghosh and Swapan K. Ghosh *J. Chem. Phys.* 134, 024502 (2011)
2. Density functional theory of size-dependent surface tension of Lennard-Jones fluid droplets using a double well type Helmholtz free energy functional. Satinath Ghosh and Swapan K. Ghosh *J. Chem. Phys.* 135, 124710(2011)



3. Density functional theory of surface tension of real fluids using a double well type Helmholtz free energy functional: application to water and heavy water. Satinath Ghosh and Swapan K. Ghosh *Mol. Phys.* 111, 589(2013)
4. Density functional theory of vapor to liquid heterogeneous nucleation: Lennard–Jones fluid on solid substrate. Satinath Ghosh and Swapan K. Ghosh *Mol. Phys.* 111, 868 (2013)
5. Spherical Seed mediated vapor condensation of Lennard-Jones fluid: A Density functional theory approach. Satinath Ghosh and Swapan K. Ghosh *J. Chem. Phys.* 139, 054702(2013)



Name : **Panchugopal Bikram**
Enrolment No. : MATH10200804002
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Extendable Endomorphisms of Factors

Abstract

This thesis is devoted to the study of weak-* continuous semigroups of unital normal * endomorphisms on arbitrary factors. It is divided into three chapters. The first chapter proposes a rephrasing of the notion of a Hilbert von Neumann module, while the last two chapters are dedicated to a class of endomorphisms and E0-semigroups on factors which we call extendable.

Hilbert von Neumann modules;

In this chapter we introduce a new way of regarding Hilbert-von Neumann modules as spaces of operators between Hilbert spaces. In a version of the Stinespring dilation theorem, we showed that the so called standard Hilbert-von Neumann bimodules associated to normal completely positive maps are singly generated in an essentially unique way. We refer to the Hilbert-von Neumann bimodule obtained by the so-called internal tensor product of two Hilbert-von Neumann bimodules as their Connes fusion.

For Hilbert-von Neumann bimodules arising from automorphisms of von Neumann algebras the Connes fusion corresponds to composition of automorphisms. Further, the isomorphism of such Hilbert-von Neumann bimodules correspond to inner conjugacy of the automorphisms.

On extendable of endomorphisms and E0-semigroups on factors;

In this chapter we examine what it means to say that equi-modular endomorphisms of a factor are extendable. We obtain several conditions on an equi-modular endomorphism, and single out one of them with a purely 'subfactor flavour' as a theorem. We use our theorem to determine when every endomorphism in an E0-semigroup on a factor is extendable { which property is easily seen to be a cocycle-conjugacy invariant of the E0-semigroup. We conclude by giving examples of extendable E0-semigroups, and by showing that the flow on the hyperfinite II1 factor is not extendable, neither is the free flow and CAR flow.

CAR flows on type III factors;

In this chapter we exhibit examples of extendable endomorphisms on factors of type III. We show that the CAR flows which are E0-semigroups on type III factor arising from quasi free states, are not extendable. We deduce that CCR flows and CAR flows are not cocycle conjugate on type III factors, unlike type I factor.

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1. Published: Hilbert von Neumann modules, with Kunal Mukherjee and R. Srinivasan and V. S. Sunder, Communications in Stochastic Analysis : Volume 6, no. 1, (March 2012).
2. Accepted: On extendability of endomorphisms and of E0-semigroups on factors, with Masaki Izumi, R. Srinivasan and V.S. Sunder accepted at the Kyushu Journal of Mathematics.
3. Preprint: Non-extendable E0-semigroup on III factors, arXiv:1304.4341 [math.OA].



Name : **Rameswar Singh**
Enrolment No. : PHYS06200704018
Constituent Institute : Institute for Plasma Research, Gandhinagar
Title : Momentum Transport : Intrinsic Rotation and Zonal Flows in Microturbulence in Tokamaks

Abstract

Microturbulence driven by equilibrium density and temperature gradients is responsible for cross field transport of particles and energy deteriorating plasma confinement in tokamaks. Mean shear flows tend to reduce energy and particle transport by enhancing the turbulence decorrelation. These flows can be either externally driven or can be self-generated by turbulence. Self-generated flows can appear at macroscopic scale and mesoscopic scale. Intrinsic toroidal and poloidal rotation without external momentum source belong to the first category while zonal flows in poloidal and toroidal direction belong to the second category. Self generated intrinsic rotation and zonal flows can be viewed as different manifestations of momentum transport in turbulence. This thesis deals with certain features of momentum transport in ion temperature gradient (ITG) driven microturbulence leading to generation of intrinsic rotation and zonal flows using mean field theory. Analytical calculations are mostly performed in sheared slab geometry and numerical simulations are performed in local flux tube geometry using the gyrokinetic turbulence code GENE.

Residual stress is identified as a key ingredient of intrinsic rotation drive whether it is toroidal or poloidal $\langle k_{\parallel} \rangle$ symmetry breaking drives parallel residual stress while $\langle k_r \rangle$ symmetry breaking drives poloidal stress assisted by radial fluctuating $E \times B$ velocity. This $\langle k_{\parallel} \rangle$ symmetry breaking is achieved by mean $E \times B$ shear and density gradient as a higher order ρ_s^* effect via mode shift off the rational surface. Here $\rho_s^* = \rho / L_n$ being ion sound radius and L_n being density gradient scale length. Poloidal residual stress by $\langle k_r \rangle$ symmetry breaking requires mean parallel flow shear. This leads to coupling of parallel and poloidal momentum fluxes and hence of intrinsic toroidal and poloidal rotations. In reverse shear tokamak with non-monotonic safety factor q , $\langle k_{\parallel} \rangle$ symmetry breaking does not require asymmetry of the eigenmode at the minimum of q due to quadratic variation in the poloidal magnetic field there. Polarization drift also drive parallel residual stress at a higher order in ρ_s^* by $\langle k_{\parallel} k_r \rangle$ symmetry breaking which does not require asymmetry of the eigenmode about the rational surface. However polarization drift fails to drive any poloidal stress. Linear gyrokinetic flux tube simulations show that toroidal ITG instability extend to short wavelength region when growth rates are maximized over all ballooning angles. Finite ballooning angle generates parallel residual momentum flux by breaking the symmetry of the eigenmode about the low field side (LFS) mid plane. Nonlinear simulations with macroscopic $E \times B$ shear show parallel residual momentum flux by symmetry breaking of the eigenmode about the LFS mid plane. $2D$ cross-correlation calculations show some finite spatially local but temporally non-local correlation between momentum flux and root mean square zonal flow shear, but zonal flow shear fails to generate volume averaged parallel momentum flux.

Zonal flow in the poloidal direction is well known to appear as a consequence of modulational instability of the ITG turbulence. Inclusion of electromagnetic effects show that near marginality the ratio of zonal flow growth to ITG mode growth increases with ratio of thermal pressure to



magnetic pressure whereas for larger η_i , ratio of density and temperature scale lengths, the zonal flow drive reduces due to the competition between Reynolds and Maxwell stresses. Toroidal zonal flows (TZF) get excited via modulational instability similar to poloidal zonal flow (PZF) excitation in ITG turbulence. Toroidal and poloidal zonal flow shears are coupled linearly via non-linear stresses. A 0D empirical model for time evolution of turbulence intensity, PZF shear, TZF shear, pressure gradient in a input power ramp shows that the input power threshold for $L \rightarrow H$ transition reduces with $PZF \rightarrow TZF$ coupling coefficient which depends on $\langle k_{\parallel} \rangle$ symmetry breaking mechanisms. In the strong turbulence regime coherent nonlinear structures like solitons, shocks, nonlinear wave trains appear in poloidal zonal flow field due to Reynolds stresses offered by trapped and untrapped ITG waves.

Publications

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3. Secondary instability of electromagnetic ion-temperature-gradient modes for zonal flow generation, Johan Anderson, Hans Nordman, Rameshwar Singh, Raghendra Singh, Phys. Plasmas, 18, 072306 (2011)
4. Parallel momentum transport in the neighbourhood of q_{\min} in reverse shear tokamaks, Rameshwar Singh, R. Singh, Hogun Jhang, and P.H. Diamond, Phys. Plasmas 2013 (submitted)
5. A new paradigm of coupled intrinsic toroidal zonal flow – ITG turbulence – poloidal zonal flow system, Rameshwar Singh, R. Singh, P. Kaw, Phys. Plasmas (to be submitted)
6. Coherent structures in ITG-zonal flow system, Rameshwar Singh, R. Singh, P. Kaw and P.H. Diamond, New J. Phys. 2013 (under review) Finite ballooning angle effects on ion temperature gradient driven mode and associated transports in gyrokinetic flux tube simulations, Rameshwar Singh, S. Brunner, R. Ganesh and F. Jenko, Phys. Plasmas (to be submitted)

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Name : **Madhushree Basu**
Enrolment No. : MATH10200704003
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Probability in von Neumann Algebras

Abstract

This doctoral thesis - titled 'Probability in von Neumann algebras' – is based on a few observations on applications and analogues of certain features of Probability theory in non-commutative W^* -probability spaces. It is divided in three chapters. In the first chapter, free products of certain finite dimensional W^* -probability spaces and free group factors are computed. The results in this chapter are in the form of isomorphisms between W^* -probability spaces, where the left hand side is always a free product of two W^* -probability spaces. Our idea is to find equivalent models of these two spaces inside the W^* -probability space on the right hand side and prove that (i) they are free inside the latter, and that (ii) they generate the latter.

The second chapter is devoted to associating W^* probability spaces to weighted graphs and deriving the associated finite von Neumann algebras as free products of certain von Neumann subalgebras with amalgamation over a commutative finite dimensional subalgebra. In particular, the von Neumann algebra associated to a 'flower with n petals' (i.e. a graph with a single vertex and n loops) turns out to be isomorphic to the group von Neumann algebra of the free group on n generators.

The third chapter extends a well-known minmax characterization by Ky Fan, of the sum of the k largest eigenvalues of an $n \times n$ Hermitian matrix ($k, n \in \mathbb{N}; k \leq n$), to a 'continuous' context. More precisely our version of Ky Fan's theorem gives an analogous statement of the finite dimensional result for a self adjoint element of a W^* probability space, such that the distribution of that element has no atoms. In our work, we also give an alternate proof for Ky fan's original result.

Publications

1. From graphs to free products, with Vijay Kodiyalam and V. S. Sunder, Proceedings - Mathematical Sciences: Volume 122, Issue 4 (2012), Page 547-560.
2. Some explicit computations and models of free products - Journal of the Ramanujan Mathematical Society: Vol 28, No. 1 (2013), Page 71-89
3. Continuous minmax theorems, with V. S. Sunder, e-print arXiv:1210.7581 [math. OA].



Name : **Ajit Kumar Mahendra**
Enrolment No. : ENGG01200704012
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Meshless Method for Slip Flows

Abstract

The thesis deals with the development of meshless method for slip flows based on kinetic scheme incorporating features of non-equilibrium thermodynamics. The subject involves research in the field of kinetic theory, non-equilibrium thermodynamics, kinetic schemes, meshless methods and optimization approaches.

Most of the upwind schemes fail to ensure the correct distribution of the entropy generation for each thermodynamic force. Hence it is difficult to formulate a single monolithic solver if it is to operate from low speed to hypersonic rarefied flow or from creeping flows to high speed continuum flow. The kinetic scheme developed in the thesis follows the principle of non-equilibrium thermodynamics and ensures the correct division of entropy generation for each thermodynamic force as the state update moves from one conservation state to another following the path laid down by non-equilibrium thermodynamics. It is more rational to incorporate features of non-equilibrium thermodynamics at the microscopic level and apply discretization at the Boltzmann level. A new approach to kinetic flux vector splitting method was formulated guided by the principles of non-equilibrium thermodynamics. Upwind scheme for macroscopic conservation equations in the new approach involves three steps : i) in the first step the Boltzmann equation is rendered into an upwind discretized form, ii) in the second step inviscid fluxes are obtained by taking moments of split Maxwellian distribution, iii) in the third step viscous fluxes are obtained by taking moments and full tensor contraction of split microscopic tensors. The present kinetic upwind scheme can be used to simulate the entire range from rarefied slip flow to continuum flow, creeping flow to flow with shocks as it is derived using kinetic theory incorporating phenomenological theory of non-equilibrium thermodynamics. One of the motivations of the thesis is to derive a unified wall boundary condition which satisfies non-equilibrium thermodynamics and can simulate both continuum and rarefied slip flow within Navier-Stokes equation in order to avoid extremely costly multi-scale simulation. The thesis presents novel kinetic flux vector splitting based wall boundary which uses Maxwell 's gas-surface interaction model incorporating features of linear non-equilibrium thermodynamics for effective resolution of slip phenomenon.

Recently, shape optimization using numerical methods has made rapid progress. The shape optimization procedure requires repeated grid generation after each iterative step. Most of the industrial problems have many complex components and generation of suitable grid for a complex multi-body configuration can be very tedious and intensive task and sometimes it becomes the bottleneck. In such a scenario we require a faster, simpler and robust meshless approach. The thesis presents a new meshless approach using least square approach by generating a non-symmetric cross-product matrix by suitable selection of sub-stencils such that the matrix is diagonally dominant and well conditioned. The thesis describes the novel Split-stencil Least square Kinetic upwind method for Navier-Stokes (SLKNS) solver which makes use of least squares and Kinetic Flux Vector Splitting (KFVS) scheme based on microscopic tensor splitting with kinetic wall boundary condition.



Publications

Journals and Books

1. A.K. Mahendra, R.K.Singh, G. Gouthaman, Meshless kinetic upwind method for compressible, viscous rotating flows. *Computers and Fluids* 2011; Vol.46 pp.325–332. (Research contribution : Development of novel meshless solver SLKNS using split stencil least square method and kinetic scheme.)
2. A.K. Mahendra, G. Gouthaman, R.K.Singh, Viscous Compressible Slip Flows. Part 1: Kinetic Flux Vector Splitting and its Variance Reduction form. *International Journal of Emerging Multidisciplinary Fluid Sciences*, 2011; Vol. 3, pp. 21–47. (Research contribution : Development of kinetic flux vector scheme in its variance reduced form.)
3. A.K. Mahendra, G. Gouthaman, R.K.Singh, Viscous Compressible Slip Flows. Part 2 : Meshless Solver for Rotating Slip Flows. *International Journal of Emerging Multidisciplinary Fluid Sciences*, 2011; Vol. 3, pp. 49–83. (Research contribution : Development of modified SLKNS.)
4. G.N. Sashi Kumar, A.K. Mahendra, G.Gouthaman, Multi-objective shape optimization using ant colony coupled computational fluid dynamics solver. *Computers and Fluids* 2011; Vol. 46 pp.298–305. (Research contribution : Multi-objective shape optimization method for ant colony coupled meshless solver SLKNS with adaptive L_p - dominance strategy.)
5. G.N. Sashi Kumar, A.K. Mahendra, A. Sanyal, and G. Gouthaman, A Hybrid Method for Multi-Objective Shape Optimization. *Lecture Notes in Computer Science* 6457 pp. 563–567, 2010 Springer- Verlag Berlin Heidelberg. (Research contribution : Multi-objective shape optimization method with hybrid method based on ant colony optimization and genetic algorithm using meshless solver SLKNS.)

Peer reviewed Symposia and Conferences

1. A.K. Mahendra, R.K. Singh, G. Gouthaman, Meshless kinetic upwind method for compressible, viscous rotating flows. *Conference on Numerical method for Fluid Dynamics, ICFD 2010, Reading U.K., 12-15 April 2010.* (Research contribution : Development of novel meshless solver SLKNS using split stencil least square method and kinetic scheme.)
2. A.K. Mahendra, R.K. Singh, Meshless kinetic upwind method for rotating slip flows. *12th AeSI Annual CFD Symposium, Bangalore, August 11-12, 2010.* (Research contribution : Extending the meshless solver SLKNS for slip flows using kinetic theory based method.)
3. A.K. Mahendra, R.K. Singh, G. Gouthaman, Shape optimization of stationary body under strongly rotating flows. *IUTAM Symposium on Bluff Body Flows, IIT-Kanpur, 12-16 December 2011.* (Research contribution : Development of multi-objective nonlinear simplex based method using meshless solver SLKNS and Fourier parametrization.)
4. G.N. Sashi Kumar, A.K. Mahendra, A. Sanyal, G. Gouthaman, 2D Meshless solver with a better spectral resolution. *13th AeSI Annual CFD Symposium, Bangalore, August 11-12, 2011.* (Research contribution : Development of meshless solver SLKNS with enhanced spectral properties.)

Research reports

1. A.K. Mahendra, Adaptive L_p -dominance coupled L_p metric strategy for multi objective - multicomponent problems, MDD Internal report, BARC, Trombay, Mumbai, January 2010. (Research contribution: Multi-objective methodology using adaptive L_p -dominance coupled L_p metric strategy.)



2. A.K. Mahendra, R.K. Singh, Onsager reciprocity principle for kinetic upwind method, MDD Internal report, BARC, Trombay, Mumbai, December 2010. (Research contribution: Development of kinetic model, kinetic scheme following Onsager's reciprocity principle.)
3. A.K. Mahendra, R.K. Singh, G. Gouthaman, Kinetic wall and no-slip boundary conditions for continuum flows, MDD Internal report, BARC, Trombay, Mumbai, November 2011. (Research contribution: Kinetic theory based wall boundary condition and its comparison with no-slip, Maxwell velocity slip and von Smoluchowski temperature jump for dissipative wall.)



Name : **Anubrata Das**
Enrolment No. : LIFE01200704001
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Functional Characterization of Hypothetical Proteins and their Role in Radiation Tolerance of *Deinococcus radiodurans*

Abstract

In this thesis work I have attempted to understand the role of a couple of hypothetical proteins found during this early phase of post irradiation recovery in *Deinococcus radiodurans*, a bacterium capable of withstanding high doses of ionizing radiation. And there is a keen interest to study the yet unknown mechanisms by which it is able to survive such high doses of ionizing radiation. It is now believed that both protection of biomolecules from oxidative damage and an efficient DNA repair plays a role in its ability to recover from the damage caused by ionizing radiation. In the cellular extracts of the early phase of the recovery process, an ATP inhibited nucleolytic activity was discovered but the factor involved could not be identified.

In this thesis I have used bioinformatics tools to predict the function of the hypothetical proteins present in the cellular extract and amongst them I predicted DR2417 as a nuclease and DRA0282 as a DNA end binding protein. Subsequently the ORFs for these hypothetical proteins were cloned and the recombinant proteins were expressed and purified. *in vitro* assays with purified DR2417 showed that it acts as a 3'-5' dsDNA exonuclease and a ss/dsDNA junction specific endonuclease and this activity is inhibited by ATP. Also a deletion mutant of DR2417 exhibited a debilitated phenotype. These studies form a strong case for identification of DR2417 as the factor responsible for the novel ATP inhibited nuclease seen in the cellular extracts of the early phase of recovery. Purified DRA0282 was characterized as a DNA end binding and DNA end protecting protein while deleting this gene showed that it probably plays a redundant role in the recovery process.

Overall this thesis throws light on the important roles of hypothetical proteins in the radiation resistance of *D. radiodurans* and how bioinformatics tools could be used to unravel their myriad functions.

Publications

Papers Published in Peer-reviewed International Journal

1. Das, AD and Misra, HS (2011). Characterization of DRA0282 from *Deinococcus radiodurans* for its role in bacterial resistance to DNA damage. *Microbiology (SGM)* 157: 2196-2205
2. Das, AD and Misra, HS (2012). DR2417m, a hypothetical protein characterized as a novel β -CASP family nuclease in radiation resistant bacterium, *Deinococcus radiodurans*. *Biochim. Biophys. Acta (General Subjects)* 1820:1052-1061
3. Das, AD and Misra, HS (2013). Hypothetical proteins present during recovery phase of radiation resistant bacterium *Deinococcus radiodurans* are under purifying selection. *J. Mol. Evol* 77:31-42



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1. Das A. D. and Misra H. S. "Functional characterization of a hypothetical protein from *Deinococcus radiodurans* and its role in bacterial resistance to DNA damage" in 34th All India Cell Biology Conference and symposium on quantitative biology : from molecules to cells, Abstract No. 64, p.142, December 4-6, 2010, Kolkata.
2. Das A. D. and Misra H. S. "A novel member of the beta CASP family of nuclease in involved in the survival of *Deinococcus radiodurans*" in 52nd Annual Conference of Association of Microbiologists of India (AMI-2011), Abstract No. MM111, p392, November 3-6, 2011, Punjab University, Chandigarh.]

Genbank Submission

1. D. Das and H. S. Misra (2012) *Deinococcus radiodurans* strain ATCC 13939 DR2417 gene. Accession No. JQ432552.

Award and other recognition

1. A. D. Das received Dr. Rana Memorial Best Poster Award during 52nd Annual Conference of Association of Microbiologists of India (AMI-2011), held at Punjab University, Chandigarh, November 3-6, 2011.



Name : **Vijay Kumar Charaka**
Enrolment No. : LIFE01200704005
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Characterization of Genome Partitioning System of *Deinococcus radiodurans*

Abstract

An accurate duplication and transmission of genetic information is a fundamental attribute of the life and that determines the successful inheritance of different phenotypes into daughter cells. In bacteria, the genome partitioning occurs mainly by pushing or pulling of duplicated genome toward the cell poles. This involves three core components like *cis*-element that functions like centromere in bacteria, a centromere binding protein and an actin homologue of bacterial ATPase. *Deinococcus radiodurans* R1 is a Gram positive bacterium that shows extraordinary tolerance to different DNA damaging agents. Genome of this bacterium encodes putative ParA and ParB types proteins located on each of the four genome elements. The *cis* elements are not known in the genome of this bacterium. Understanding the function of 'Par' proteins would be a step forward in knowing the mechanism(s) of chromosome segregation in this bacterium that also harbors complex genome. Here I have , for the first time, identified the *cis* elements (named *segS* elements) in the genome of *D. radiodurans* and functionally characterized one of the three *segS* i.e *segS3* for its role in plasmid stability and its interaction with cognate ParA and ParB proteins *in vivo* and *in vitro*. Enhanced stability of unstable mini-F plasmid in the presence of *segS3* and its cognate partitioning proteins, oscillation of GFP-ParA1 in *E. coli* harboring *segS3* bearing plasmid, and loss of nucleoid in *parB1*deletion mutant of *D. radiodurans*, and *in vitro* activity characterization of these elements strongly supported their roles in genome segregation. I further showed that ParA2 (ParA of chromosome II) in the absence or lower ratio of its cognate ParB (ParB2) also function beyond genome segregation i.e. in the regulation of cell division. This has been another new and novel finding from this study. Thus, I have been able to functionally characterize a complete tripartite partitioning system in chromosome I of *D. radiodurans* and also chromosome II partitioning proteins role in genome maintenance and cell division of this bacterium.

Publications

Published :

1. Charaka, V. K. and Misra, H. S. (2012) Functional characterization of chromosome I partitioning system in *Deinococcus radiodurans* for its role in genome segregation. J. Bacteriol. 194:5739-5748.
2. Charaka, V.K.umar and Misra, H.S. (2013) ParA2, A hypothetical walker type DNA binding ATPase of *Deinococcus radiodurans*, arrests septal growth by Nucleoid occlusion mechanism. J. Bioscience. 38:487-497.
3. Kota, S., Charaka, V.K.,and Misra, H.S. (2010) Characterization of an ATP-regulated DNA-processing enzyme and thermo tolerant phosphoesterase in the radioresistant bacterium *Deinococcus radiodurans*. Biochem J. 431:149-157.

Communicated:

1. Kota,S., Charaka,V.K.,Ringgaard,S., Waldor,M.K. and Misra,H.S (2013)PprA has a role in maintenance of damaged genome in *Deinococcus radiodurans*, pLOS one (*Under revision*)



Name : **Trilochan Bagarti**
Enrolment No. : PHYS07200604031
Constituent Institute : Institute of Physics, Bhubaneswar
Title : A Theoretical Study of Formation of Clusters at Nanoscale Using Reaction-Diffusion Models in One and Two Dimensions

Abstract

A theoretical study of formation of cluster at nanoscale using reaction-diffusion models in one and two dimensions

In this thesis we present a theoretical study of reaction-diffusion models in the presence of disorder. The motivation of this work comes from experiments in which Ge is deposited on Si surfaces. From the experiments it was found that clusters were preferentially formed at the locations of surface defects on Si surfaces. Through these reaction-diffusion models the growth process of Ge clusters on Si surfaces are studied. It is found patterns formed are qualitatively similar to those observed in the experiments. So, we establish through this work that these patterns are primarily induced by surface defects and domain boundaries.

In the first part of the thesis we study the cluster formation by linear reaction-diffusion model. The cluster formation process is approximated by a first order reaction in the presence of surface defects. The surface defects are assumed as isolated regions on the Si surface where the reactions take place. However, away from the defects there is only diffusion and no reactions can occur. Diffusion coefficients. The coupled reaction-diffusion equations are solved by Green's functions and regular perturbation technique in the abstract vector space. The model qualitatively explains the observed phenomena.

In the second part of the thesis we consider the formation of cluster in the presence of exclusion. The origin of exclusion is related to non-bonding interactions between the particles. In any volume element only a finite number of particles can be accommodated. So, when the number of cluster particles in the volume element increases, adatoms and/or cluster particles repel one another. The adatom-cluster exclusion is incorporated into the reaction-diffusion equations through a repelling force proportional to the gradient of the concentrations. This exclusion terms are derived from the microscopic principle using master equation. Nonlinear term appears in the reaction-diffusion equations which consists of coupling of the concentration of one species with the gradient of the other species. For the cluster formation in the vicinity of a surface defects, we further consider an algebraic nonlinear reaction process in which many adatoms react to form a cluster.

In the limit when exclusion effect is weak we find a linearized reaction-diffusion equation. The linear equation gives us very important insight into the process. We find that due to the presence of exclusion an extra drift term appears in the reaction-diffusion equations. For the adatoms the drift velocity is outward from the location of the point defect where as for the cluster particles it is directed into the defect site. Furthermore, it also breaks the symmetry of the reaction terms by effectively modifying the reaction rates. The width of the cluster concentration profile is found to be decreasing with increasing exclusion strength and decreasing nonlinearity. In two dimension it is found that the mean concentration decreases with nonlinearity and exclusion. The most interesting conclusion that we draw from this model is that exclusion and algebraic nonlinearity both suppress the formation of clusters.



We have further studied the effect of self-exclusion in reaction-diffusion process to study trapping reaction problem. Perturbative solution to the reaction-diffusion is calculated upto second order in reaction rate. Stretched exponential law is derived in the presence of exclusion.

We finally conclude that reaction-diffusion models in inhomogeneous media can be used to describe the formation of clusters at nanoscales in the presence of surface defects of any topology, step edges and domain boundaries. The surface defects are modeled as reaction centers in the reaction-diffusion model having various topologies. We find that models considered, albeit minimal in nature, are quite good in explaining qualitatively the formation of clusters. In the nonlinear model we have investigated the effect of exclusion and nonlinearity in the cluster formation process. We draw the most important conclusion that exclusion and nonlinearity both have a suppressing effect in the formation of clusters.

Publications

1. Patterns in Ge cluster growth on clean and oxidized Si(111)-(7×7) surfaces Anupam Roy, Trilochan Bagarti, K. Bhattacharjee, K. Kundu, B.N.Dev, Surf. Sci. 606, 777 (2012).
2. A reaction diffusion model of pattern formation in clustering of adatoms on silicon surfaces Trilochan Bagarti, Anupam Roy, K. Kundu, B.N. Dev, AIP Advances **2**, 042101 (2012).
3. The effect of exclusion on nonlinear reaction diffusion system in inhomogeneous media Trilochan Bagarti, Anupam Roy, K. Kundu and B. N. Dev, (to be submitted)
4. Universality in shape evolution of Si_{1-x}Gex structures on high index Silicon surfaces J. K. Dash, T. Bagarti, A. Rath, R. R. Juluri and P. V. Satyam, EPL **99** 66004 (2012).



Name : **Veerendra Kumar Sharma**
Enrolment No. : PHYS01201004017
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Stochastic Molecular Dynamics in Picoseconds Time Scale :
Neutron Scattering and Molecular Dynamics Simulations Studies

Abstract

The thesis is devoted to the study of molecular dynamics in various complex systems including self-assembled aggregates like micelles and fluids confined in restricted geometries using quasi elastic neutron scattering (QENS) and computer simulation techniques. Both techniques are used in tandem to unravel complex dynamical features at wide range of time scales from nanoseconds to picoseconds, and a length scale from angstroms to nanometers.

In this thesis, the first chapter deals with basic theoretical aspects of QENS and computer simulation. The next four chapters of the thesis consist of studies of dynamics of surfactants in self assembled micelles as well as in solid crystalline form. Detailed dynamical landscapes of various ionic micelles such as SDS, CTAB, etc. have been investigated using various QENS spectrometers covering wide range of time scales. It is found that QENS data have contributions from three distinct motions: (i) global motion of micelles (ii) segmental motion of monomer and (iii) fast torsional motion. QENS data recorded over a wide dynamical range have been described consistently by suitable modeling and considering all these motions. Results are in accordance with findings from simulation studies. Effect of molecular architecture (different chain lengths, additional phenyl ring) of the monomer on dynamics of the micelles is also investigated and a correlation between dynamics and microstructure of the micelles is established. It is also of interest to check whether these surfactants in solid phase show any dynamical motion or not. With that view, dynamics of solid SDS powder has been investigated and a temperature dependent transition from uniaxial reorientation to 'micelle like' dynamical behavior is observed at higher temperatures.

Knowledge of the effect of confinement on the dynamical behaviour of fluids in nanoscopic regimes is useful in wide spread applications such as energy storage, molecular sieving, waste management and water filtration etc. Dynamics of guest molecules (water, hydrocarbons, etc.) in various nanoporous frameworks (polyimide membranes, zeolites, Prussian blue analogues) have been investigated in details. Chapter six describes the dynamics of water in polyamide membranes and Prussian blue analogues. It is found that translational motion of water confined in these membranes gets modified compared to bulk water whereas rotational motion remains unaltered. In case of Prussian blue analogues, dynamics of water is found to be highly dependent on its location in the crystal lattice. Evolution of dynamics with temperature has been described and the contributions from different water molecules in the lattice are evaluated quantitatively. The seventh chapter discusses the effect of zeolitic host structure on the dynamics of adsorbed hydrocarbon. Both translational as well rotational motions of propylene are found to be affected depending on the zeolite structures. Various striking observations such as preferred orientation, libration motion, have been observed which are highly dependent on the host topology. The last chapter summarizes the present work and also provides directions for future work based on the results presented in this thesis.



Publications

1. Dynamics in Anionic Micelles: Effect of Phenyl Ring V. K. Sharma, S. Mitra, M. Johnson and R. Mukhopadhyay, *J. Phys. Chem. B* 117 (2013) 6250.
2. Dynamics of Molecular Species in Confined Geometry V. K. Sharma, S. Mitra and R. Mukhopadhyay, *J. Phys. Soc. Japan* 82 (2013) SA006
3. Dynamical features in Cationic Micelles of Varied Chain Length V. K. Sharma, S. Mitra, V. Garcia Sakai and R. Mukhopadhyay, *J. Phys. Chem. B* 116 (2012) 9007.
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18. Diffusion of hydrocarbon in Zeolite and Effect due to Pore Topology: Neutron Scattering and MD Simulation Studies Mitra, V. K. Sharma, S.L. Chaplot and R. Mukhopadhyay (Submitted)
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Name : **Diganta Das**
Enrolment No. : PHYS10200804004
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Model Independent Extraction of New Physics from Hadronic
Uncertainties in $B \rightarrow K^* l^+ l^-$ Decay

Abstract

The discovery of New Physics, using weak decays of mesons is difficult due to intractable strong interaction effects needed to describe it. We show how the multitude of related observables obtained from $B \rightarrow K^* l^+ l^-$, can provide many new clean tests of the Standard Model. The hallmark of these tests is that several of them are independent of the unknown form factors required to describe the decay using heavy quark effective theory. We show how any observable can be expressed independent of these Isgur—Wise form factors. We derive signals of new physics in terms of relation between observables that is free of form factors and Wilson coefficients, the violation of which will be an unambiguous signal of New Physics. We also derive other relations between observables and form factors that are independent of Wilson coefficients and enable verification of hadronic estimates. We find that the allowed parameter space for observables is very tightly constrained in Standard Model, thereby providing clean signals of New Physics. The relations derived will provide unambiguous signals of New Physics if it contributes to these decays.

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Preprint

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Name : **Swati Panigrahi**
Enrolment No. : LIFE05200704002
Constituent Institute : Saha Institute of Nuclear Physics, Kolkata
Title : Role of Hydrogen Bonding Interactions in Biologically Important Macromolecules

Abstract

Hydrogen bonds are the key factors for stabilizing the range of macromolecules such as proteins, RNA, DNA, carbohydrates and play significant role in molecular recognition process. We have studied the structure and energetic of various hydrogen bonded systems to predict their applications in various nano-bio interface through quantum chemical analysis. It has been observed that a number of base pairing geometry between the four nucleobases of RNA are possible. We have optimized all these basepairs, which are stabilized by two hydrogen bonds, by different quantum chemical methods and determined the strengths of each type of the hydrogen bond, namely N-H...O, N-H...N, O-H...N, C-H...O, C-H...N. We observed sufficient overlapping of the molecular orbitals in case of polar hydrogen bonded systems. Noncanonical basepairs seem to have more number of acceptor and donor sites for the accessible of other small molecules, ligands, drugs etc. as compared to the canonical ones. We have also observed that some of the noncanonical basepairs undergo conformational changes during optimization, or can adopt different geometry. Probably they can act as conformational switch in the complex RNA molecule.

Carbonaceous materials such as grapheme and carbon nanotube T) can act as efficient carrier for drug delivery. We observed they have strong binding interactions with the nucleobases and nucleosides, from analysis using dispersion corrected density functional theory, where π - π stacking interaction is also considered. The two edges of grapheme are observed to interact differently with the water molecule through weak C-H...O hydrogen bonds. We observed that zig-zag edge is more hydrophilic than the arm-chair edge. The importance of capping for stabilization of gold nanoparticle and importance of hydrogen bonding for interaction of the gold nanoparticle with other drug molecules have been also studied through density functional theory with relativistic corrections.

Publication in refereed journals:

1. Roy, S. Panigrahi, M. Bhattacharyya and D. Bhattacharyya (2008) Structure, stability, and dynamics of canonical and noncanonical base pairs: quantum chemical studies, *J. Phys. Chem. B*, 112, 3786-96.
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1. Comparison of B3LYP/6-31G** and HF/cc-pVDZ methods in structure and energetics of hydrogen bonded nucleotide basepairs , presented at —National Symposium on Quantum Chemistry, soft computing and Optimization , IACS, Kolkata, April 4-5, 2008.
2. Variation of sugar pucker in RNA structures: Crystal database and quantum chemical studies , poster presented at —National Symposium on Cellular and Molecular Biophysics, CCMB, Hyderabad, January 22-24, 2009.
3. Wetting Properties of Planar Nano Graphene: A AFM and Quantum Chemical Approach , poster presented at — International Symposium on Facets of Weak Interactions in Chemistry, at Saha Institute of Nuclear Physics, Kolkata, organized by Calcutta University, from 13-15 January, 2011.
4. Binding of nucleobases with wrinkled graphene surface: Dispersion corrected DFT approach and AFM studies , poster presented at —2nd International Conference on Advanced Nanomaterials and Nanotechnology (ICANN-2011) , Dec 8-10, 2011 at Indian Institute Of Technology, Guwahati.
5. Study of Interactions of Nanomaterials with Nucleotides: A Quantum Chemical Approach , poster presented at — Recent Advances in Chemical and Physical Biology at Saha Institute of Nuclear Physics, Kolkata, organized by Saha Institute of Nuclear Physics (SINP), India and The Mechanobiology Institute (MBI), NUS, Singapore, from 5-7 March, 2012.

Schools/Symposium attained

1. International Conference on Physics Biology Interface , December 13-16, 2009, at Saha Institute of Nuclear Physics, Kolkata, India
2. One day satellite symposium on —Recent trends in Peptide research , on January 8, 2010 at Bose Institute Kolkata
3. Schools on Computational Techniques in Soft Matter 2010 (CTAM10), December 6-10, 2010, at S.N. Bose National Centre of Basic Sciences, Kolkata.



Name : **Vikram Sagar**
Enrolment No. : PHYS06200704006
Constituent Institute : Institute for Plasma Research, Gandhinagar
Title : Laser Driven Acceleration of Charged Particles in Vacuum

Abstract

This thesis is devoted to the study of laser driven acceleration of charged particles in vacuum. The following two schemes of particle acceleration namely: “the laser driven auto-resonant acceleration” and “direct acceleration of particles by a focused laser field” have been theoretically investigated. It has been further shown that these two schemes of particle acceleration can be easily combined together to enhance the efficiency of the acceleration scheme.

The scheme of laser driven auto-resonant particle acceleration is of great interest, as in this scheme the acceleration rate is higher and radiation losses are lower as compared to other schemes of particle acceleration. In the laser driven auto-resonant scheme, the particle is subjected to the combined field of laser and a static axial magnetic field. The particle acceleration is achieved as a result of self sustained initial resonance between the wave frequency and cyclotron frequency of the particle. This resonance is maintained due to a precise cancellation of the relativistic mass effect due to the motion along the transverse direction which lowers the cyclotron frequency of the particle and a Doppler effect along the longitudinal direction, as result of which the frequency of the wave as seen by the particle is lower than the actual wave frequency. The renewed interest in this scheme is due to the observation of ultra high magnetic fields in the simulations as well as in the laboratory experiments pertaining to intense laser solid interaction. The observed magnetic fields are typically of the order of hundreds of mega-gauss and in general are found to be in turbulent state. However, in some of the cases, the fields are found to be coherent for a longer duration time compared to the time of interaction between the laser pulse and particle. Thus a detailed analytical as well as numerical understanding of the scheme is required to optimize the use of these magnetic field for experimental realization of the scheme. In this thesis, the particle acceleration is analytically and numerically studied using a “Gaussian” shaped temporal profile for the first time; this profile allows an unambiguous comparison between the analytical and numerical results. It is shown that particle with significant energy gain can be obtained for an optimum choice of parameters in terms of axial magnetic field, pulse width and peak laser intensity.

In the other scheme, the particle is accelerated by subjecting it to a focused laser field. For a focused laser, there is asymmetry in configuration of electric as well as the magnetic fields, which are found to be strongest near the focal point and grows weaker while moving away from it. As a result of this asymmetry, the weaker laser field far away from the focus is not able to extract back the energy transferred to the particle by the laser closer to the focus and hence a net energy is imparted to the particle along the direction of propagation of laser. For a range of parameters the energy gain is obtained by numerically solving the equation of motion. These numerical results are compared with the analytical results which are obtained using a newly derived adiabatic formulation. The adiabatic formulation is derived using canonical transformation and Lie-transform perturbation method. It is shown that the analytical description provides good quantitative estimates of the numerical results. From these estimates, the optimum conditions for maximum energy gain of the particle are determined. The theoretical understanding of the above two acceleration schemes is used to describe a new scheme of particle acceleration. In this scheme the particle is subjected to the combined field of focused finite duration laser and static axial magnetic field. It is shown that for suitable choice of parameters, the scheme results in efficient acceleration of particles.



Publications

1. Exact analysis of particle dynamics in combined field of finite duration laser pulse and static axial magnetic field , Vikram Sagar, Sudip Sengupta and P Kaw, Phys. Plasmas 19, 113117 (2012);
2. Adiabatic Formulation For Charged Particle Motion Inhomogeneous Electro- magnetic Field; Vikram Sagar, Sudip Sengupta, P Kaw, Journal Laser And Particle Beams, Vol. 31, issue 03, pp. 439-455 (2013);
3. Effect of Laser Pulse Polarization and Focusing On Particle Acceleration By Cy- clotron Au Resonance Vikram Sagar, Sudip Sengupta, P Kaw, Journal Laser And Particle Beams to be submitted.



Name : **Madhava B. Malla**
Enrolment No. : CHEM01200604036
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Title : Synthesis and Evaluation of $^{99m}\text{Tc}(\text{CO})_3$ Complexes of 'Differently Substituted Nitroimidazoles as Agents for Targeting Tumor Hypoxia

Abstract

The present thesis reports the syntheses of several nitroimidazole-bifunctional chelate conjugates and their subsequent radiosyntheses, using the precursor complex $[\text{}^{99m}\text{Tc}(\text{CO})_3(\text{H}_2\text{O})_3]^+$ for the detection of tumor hypoxia. The logical conclusions derived from the in vivo evaluation of these complexes in suitable tumor bearing animal models were further utilized to develop new/modified hypoxia targeting agents with better efficacy. The thesis consists of four chapters and the contents of each of the chapter are summarized below.

Chapter 1 of this thesis introduces basic concepts such as hypoxia, existing techniques for the detection of hypoxia and an overview of radiopharmaceuticals for the detection of hypoxia. Characterisation methods and other procedures which are commonly employed in different chapters of this thesis were also mentioned in this chapter.

Chapter 2 of this thesis attempts to analyze the influence of important molecular properties of nitroimidazole complexes, such as single electron reduction potential (SERP), lipophilicity and overall charge, on the efficacy of the complex to detect hypoxic cells. Nine different nitroimidazole- $^{99m}\text{Tc}(\text{CO})_3$ complexes were evaluated in fibrosarcoma tumor bearing Swiss mice. The results obtained were compared with that of standard agent $[\text{}^{18}\text{F}]\text{Fluoromisonidazole}$ ($[\text{}^{18}\text{F}]\text{FMISO}$), evaluated in the same animal model. The study clearly demonstrated that the clearance profile of the radiotracer from blood, which depends on the lipophilicity of the complex, is extremely important in deciding the efficacy of the radiotracer to detect hypoxic cells.

The 2-nitroimidazole-IDA- $^{99m}\text{Tc}(\text{CO})_3$ complex, evaluated in Chapter 2, showed the highest uptake and retention in tumor. However, the complex also showed significant uptake and slow clearance from liver which limited its utility to image tumors in upper abdominal region.

In Chapter 3, in an attempt to improve the liver clearance, the propylene spacer in the original complex was replaced with an ether spacer. The biological evaluation of the modified complex showed clearance of activity from liver was improved, as expected, while retaining its tumor uptake characteristics.

Chapter 4 describes the synthesis, radiolabeling and biological evaluation of a ^{99m}Tc -analogue of $[\text{}^{18}\text{F}]\text{FMISO}$, which is a PET radiopharmaceutical, currently in clinical use for imaging tumor hypoxia. The misonidazole- $^{99m}\text{Tc}(\text{CO})_3$ complex evaluated herein proved to be the best among various nitroimidazole complexes. Though this complex was not at par with $[\text{}^{18}\text{F}]\text{FMISO}$, this study provided valuable insights which could significantly help in deciding better ^{99m}Tc -based hypoxia imaging radiopharmaceuticals

In this thesis the attempt to understand the influence of various molecular properties on the efficacy of nitroimidazole complexes of ^{99m}Tc was achieved to a significant extent. The conclusions drawn from the study has shown the significance of controlling the clearance of the radiotracer from blood and a possible method of achieving it by controlling the lipophilicity.



Publications

1. On the structural modification of 2-nitroimidazole- $^{99m}\text{Tc}(\text{CO})_3$ complex, a hypoxia marker, for improving in vivo pharmacokinetics Mallia, M.B., Kumar, C., Mathur, A., Sarma, H.D., Banerjee, S. (2012) *Nuclear Medicine and Biology*, 39 (8), pp. 1236-1242.
2. Synthesis and evaluation of 2-, 4-, 5-substituted nitroimidazole- iminodiacetic acid- $^{99m}\text{Tc}(\text{CO})_3$ complexes to target hypoxic tumors Mallia, M.B., Subramanian, S., Mathur, A., Sarma, H.D., Venkatesh, M., Banerjee, S. (2010) *Journal of Labelled Compounds and Radiopharmaceuticals*, 53 (8), pp. 535-542.
3. Synthesis, radiolabeling and evaluation of $^{99m}\text{Tc}(\text{CO})_3$ -labeled misonidazole analogue to target tumor hypoxia (Abstract) Mallia, M.B., Mathur, A., Banerjee, S., Sarma, H.D., Venkatesh, M. (2010) *Nuclear Medicine and Biology*, 37 (6), pp. 682-683.
4. On the isolation and evaluation of a novel unsubstituted 5-nitroimidazole derivative as an agent to target tumor hypoxia Mallia, M.B., Subramanian, S., Mathur, A., Sarma, H.D., Venkatesh, M., Banerjee, S. (2008) *Bioorganic and Medicinal Chemistry Letters*, 18 (19), pp. 5233-5237.



Name : **Prem Prakash Pandey**
Enrolment No. : MATH10200604008
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Some Problems in Number Theory

Abstract

This is abstract of work done for the degree of Doctor of Philosophy of Homi Bhabha National Institute. We have considered three different problems and some progress is reported on each.

The first problem is study of "distribution of l^{th} residue symbols", generalizing the work of R. Balasubramanian, R. Thangadurai and F. Luca. The second problem considered is "Catalan's conjecture over Number fields".

We achieve some preliminary result in this direction but are quite far from solving the problem completely even for quadratic imaginary number fields with class number one. The third work done is an improvement on Kneser's theorem on providing "structure" on sets with small "doubling".

Publications

1. (joint with R. Balasubramanian) Density of Primes in l^{th} Power Residues, accepted in Proceeding of Indian Academy of Sciences.
2. (joint with R. Balasubramanian) Catalan's Equation for even primes over quadratic fields (submitted) <http://arxiv.org/abs/1112.2688>.
3. (joint with R. Balasubramanian) Catalan's conjecture Revisited, In Prepa- ration.
4. (joint with R. Balasubramanian) A Remark on a Theorem of Deshouillers and Freiman (Submitted).



Name : **K. Saravanakumar**
Enrolment No. : PHYS02200704017
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Rheological Studies on Ionic Liquid Dispersions of Surfactant and Nanoparticles

Abstract

This thesis presents the rheological studies on ionic liquid, BmimCl, and its dispersions of surfactant, SDS with different concentrations of LiCl salt as a function of temperature. It also presents the rheological studies on another ionic liquid, EmimTFSI dispersions of silica nanoparticles at different temperatures.

Rheological studies have revealed that the ionic liquid BmimCl behaves as viscoelastic liquid at lower temperatures ($\leq 80^\circ\text{C}$), whereas it behaves like a structured liquid at higher temperatures ($\geq 100^\circ\text{C}$).

Rheological studies have been carried out on the ionic liquid, BmimCl dispersions of surfactant, sodium dodecyl sulfate having different concentrations of the salt, lithium chloride as a function of temperature. Upon increasing the temperature a transition from viscoelastic ($< 80^\circ\text{C}$) to weak gel state ($> 80^\circ\text{C}$) is observed for ionic liquid dispersions having 4.45 wt% SDS and 18.7% LiCl. Small angle neutron scattering studies revealed the presence of wormlike micelles. The weak gel state observed at high temperatures arises due to the disintegration of the association structures of the ionic liquid along with concomitant formation of micellar network structures.

Silica-ionic liquid nanocomposite (SINC) has been prepared by dispersing different amounts of silica nanoparticles in Emim TFSI ionic liquid. Dynamic rheological studies on SINC samples with different concentrations of silica nanoparticles have shown that the nanocomposite behaves as weak gel at lower concentrations ($< 3\text{wt}\%$) whereas it behaves as gel at higher concentrations ($\geq 3\text{wt}\%$). Upon increasing the temperature weak gel samples behaves as gels whereas gel samples continue to behave as gels with increased gel strength.

Publications

Publications in Journals

1. "Thermo-reversible Viscoelastic to Weak Gel transition in a micellar-ionic liquid with salt", K. Saravanakumar, B. V. R. Tata and V.K. Aswal, Colloids and Surfaces A, 414 (2012) 359-65.
2. "Abnormal Thermo-rheological behaviour observed for Silica Ionic Liquid Nanocomposites", K. Saravanakumar and B. V. R. Tata (Manuscript under preparation)
3. "Rheological behaviour of ionic liquid BmimCl as a function of temperature", K. Saravanakumar and B. V. R. Tata (Manuscript under preparation).

Publications in Conference proceedings

1. "Thermo-reversible Viscoelastic to Weak Gel transition in a micellar-ionic liquid solution", K Saravanakumar, B. V. R. Tata and K. A. Venkatesan, DAE-Solid State Physics Symposium, Editors, A.K. Rajaraman, A.B. Garg and G. P. Kothiyal, Vol.54, p. 257-8, 2009, Vadodara, India.
2. "Effect of Temperature on Soft Glassy Behaviour of Silica-Ionic Liquid Nanocomposite" K. Saravanakumar and B. V. R. Tata, IEEE Xplore Conference Publications, ICONSET (2011) 40-43.



Presentations in Conferences

1. "Rheological characterization of Sol and Gel states in amicellar-ionic liquid solution", K. Saravanakumar, B. V. R. Tata, J. Brijitta and K. A. Venkatesan, International Conference on Sol-Gel processes for Advanced Ceramics (SGPAC), October 11-14, 2009, Kalpakkam, India.
2. "Thermo-reversible Viscoelastic to Weak Gel transition in a micellar-ionic liquid solution", K. Saravanakumar, B. V. R. Tata and K. A. Venkatesan, DAE-Solid State Physics Symposium (SSPS), December 14-18, 2009, Vadodara, India.
3. "Rheological studies on micellar-ionic liquid as a function of temperature", K. Saravanakumar, B. V. R. Tata and K. A. Venkatesan, SERC School-cum-Symposium on Rheology of Complex Fluids, January 04-09, Chennai, India.
4. "Effect of Temperature on Soft Glassy Behaviour of Silica-Ionic Liquid Nanocomposites", K. Saravanakumar, B. V. R. Tata and K. A. Venkatesan, International Conference on Nanoscience, Engineering and Technology, November 28-30, 2011, Chennai, India.



Name : : **T. Sathyanarayana Annam**
Enrolment No. : : PHYS02200704012
Constituent Institute : : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : : Effect of Pressure and Magnetic Field on the Resistance Behaviour of Transition Metal Pnictides (BaFe_2As_2 BaMn_2As_2 and FeSb_2)

Abstract

Chemical substitution and applied pressure are employed to perturb three transition metal pnictide systems exhibiting different magnetic ground states. The first example pertains to the study of the change in the ground state properties of BaFe_2As_2 that stabilizes in a Spin Density Wave (SDW) ground state. This SDW state is progressively modified as Co is substituted into the system, bringing in superconductivity. Here we study the anisotropic magnet-transport in single crystals in the SDW and superconducting regimes. The second example examines the case of an insulating G-type anti-ferromagnet, BaMn_2As_2 single crystal. Under pressure, metallicity is induced, with a hint of a possibility of superconductivity. Chemical substitution of BaMn_2As_2 also brings to bear a metallic ground state. The third example is that of a Kondo insulating FeSb_2 , where the compensated moment on Fe, is disrupted by the application of pressure and chemical substitution. Here again metallization under pressure and substitution results in exotic magneto resistance behaviour

The salient features of present thesis are

- the measurements are done on single crystals synthesized in house
- anisotropy of resistance behavior in the SDW state of $\text{BaFe}_{2-x}\text{Co}_x\text{As}_2$ single crystals in magnetic field (0 to 12T) applied parallel and perpendicular to face of the crystal has been measured.
- Upper critical field (H_{c2}) has been determined using the onset of the superconducting transition temperature from resistivity measurements in fields parallel to the face of crystal ($H \parallel ab$) and perpendicular to it ($H \parallel c$). The temperature variation of anisotropy in the upper critical field γ defined as H_{c2}^{ab}/H_{c2}^{ab} is then evaluated.
- Metallisation of single crystals of BaMn_2As_2 has been measured by temperature dependent resistivity measurements carried out under pressure from 0 to 8 GPa.
- High pressure XRD from 0 to 10 GPa is carried out at room temperature.
- Results of XRD on polycrystals of $\text{Ba}_{1-x}\text{Yb}_x\text{Mn}_2\text{As}_2$ and $\text{BaMn}_2\text{As}_{2-x}\text{P}_x$ give evidence for their substitution and show tendency to metallise.
- High pressure resistivity measurements on poly crystals of pristine FeSb_2 in the temperature point to metallization under pressure.
- Although by Ni substitution in FeSb_2 the semiconducting gap shows an increase, defects states in the gap tend to delocalize, leading to a positive temperature co-efficient of resistance behaviour. Application of magnetic field in the range 0 to 12 T, results in localization of these states.

Publications

Publications included in Thesis

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Solid State Communications 150, 1940 (2010)
3. Pressure induced Metallization of $BaMn_2As_2$ A. T. Satya, Awadhesh Mani, A. Arulraj, N. V. Chandra Shekar, K. Vinod, C. S. Sundar, and A. Bharathi Phys. Rev. B 84, 180515(R) (2011)
4. The pressure induced insulator to metal transition in $FeSb_2$ Awadhesh Mani, J Janaki, A T Satya, T Geetha Kumary and A Bharathi J. Phys.: Condens. Matter 24 , 075601 (2012)
5. Influence of Ni doping on the electrical and structural properties of $FeSb_2$ J Janaki, Awadhesh Mani, A.T.Satya, T Geetha Kumary , S Kalavathi and A Bharathi Phys. Status Solidi B 249, No. 9, 1756–1760 (2012)

Publications not included in Thesis

1. Superconducting $Fe_{1+δ}Se_{1-x}Te_x$ thin films: growth, characterization and properties T Geetha Kumary, Dipak Kumar Baisnab, J Janaki, Awadhesh Mani, A T Satya, R M Sarguna, P K Ajikumar, A K Tyagi and A Bharathi Supercond. Sci. Technol. 22, 095018 (2009)
2. Critical properties of superconducting $Ba_{1-x}K_xFe_2As_2$ A. Bharathi , Shilpam Sharma, S. Paulraj, A.T. Satya, Y. Hariharan and C.S. Sundar Physica C 470, 8 (2010)
3. Superconductivity in Ru-substituted polycrystalline $BaFe_{2-x}Ru_xAs_2$ Shilpam Sharma, A. Bharathi, Sharat Chandra, V. Raghavendra Reddy, S. Paulraj, A. T. Satya, V. S. Sastry, Ajay Gupta, and C. S. Sundar Phys Rev B 81, 174512 (2010)
4. Intricacies of strain and magnetic field induced charge order melting in $Pr_{0.5}Ca_{0.5}MnO_3$ thin films Dipak Kumar Baisnab n, T. Geetha Kumary, A.T. Satya, Awadhesh Mani, J. Janaki, R. Nithya, L.S. Vaidhyanathan, M.P. Janawadkar, A. Bharathi Journal of Magnetism and Magnetic Materials 323, 2823 (2011)
5. Superconducting and critical properties of $PrOFe_{0.9}Co_{0.1}As$: effect of P doping Shilpam Sharma, Jai Prakash, Gohil S Thakur, A T Satya ,A Bharathi, A K Ganguli, and C S Sundar Supercond.Sci. Technol. 24, 065020(2011)
6. Vibrational, magnetic, and dielectric behavior of La-substituted $BiFeO_3$ - $PbTiO_3$ K. K. Mishra, A. T. Satya, A. Bharathi, V. Sivasubramanian, V. R. K.Murthy, and A. K. Arora J Appl Phys 110, 123529 (2011)

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2. Strain enhanced charge order melting in $Pr_{0.5}Ca_{0.5}MnO_3$ thin films Dipak Kumar Baisnab, T.Geetha Kumary, A.T.Satya, Awadesh Mani, J.Janaki, R.Nithya, L.S.Vaidhyanathan, M.P.Janawadkar and A.Bharathi AIP Conf Proc. 1347,199 (2011)
3. Effect of hole doping on magnetic properties of $GdBaCo_2O_{5.5}$ N. Thirumurugan, A.T.Satya, J.Janaki and A.Bharathi AIP Con Proc. 1347, 274-277 (2011)



4. Dirac Cone States in Ru doped BaFe_2As_2 as observed by Magneto Resistance measurements. A. T. Satya, K. Vinod, Shilpam Sharma, C. S. Sundar and A. Bharathi 56th DAE SSPS 2011, AIP Conf. Proc. 1447, 901 (2012);
5. Metal – Insulator transition upon Ni substitution in $\text{Fe}_{1-x}\text{Ni}_x\text{Sb}_2$ Kondo Insulating system J. Janaki, Awadhesh Mani, A. T. Satya, T. Geetha Kumary, S. Kalavathi and A. Bharathi 56th DAE SSPS 2011, AIP Conf. Proc. 1447, 929 (2012)
6. Phase Diagram of Ru Doped BaFe_2As_2 . Vinod, Shilpam Sharma, A. T. Satya, C. S. Sundar and A. Bharathi 56th DAE SSPS 2011, AIP Conf. Proc. 1447, 889 (2012)



Name : **Jammu Ravi**
Enrolment No. : CHEM02200804009
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Development of Advanced Reagents and Methods for the Separation of Actinides from Nitric Acid Medium

Abstract

Partitioning of trivalent actinides and transmutation into stable innocuous products is being considered as a viable method for the safe management of high-level liquid waste (HLLW) arising from reprocessing of spent nuclear fuels. Among the various reagents studied for partitioning of trivalent actinides from HLLW by liquid-liquid extraction, diglycolamides (DGAs) are emerging as promising candidates. The DGA derivatives such as tetra-octyl diglycolamide (TODGA) and tetra 2-ethylhexyl diglycolamide (TEHDGA) received much attention in the recent past. However, their low metal loading capacity leading to third phase formation and co-extraction of undesirable metal ions limit their application for the industrial scale separations.

Present work involves the synthesis of some novel unsymmetrical diglycolamides (UDGAs), and their evaluation for the partitioning of minor actinides from HLLW. The alkyl group attached to the amidic nitrogen atom of UDGAs was to obtain desirable properties for efficient extraction of trivalents without leading to third phase formation and poor extraction of undesirable metal ions etc. In addition, a new approach namely "Single-cycle process for the Minor Actinide partitioning using completely incinerable ReagentTs(SMART)" for direct separation of trivalent actinides from HLLW has been developed by using a mixture of UDGA and diglycolamic acid. Since the UDGAs are proposed for solvent extraction applications of HLLW, the radiation stability of UDGAs were evaluated under process conditions. The study clearly indicated that the UDGAs reported in the present study are superior candidates for process scale applications as compared to the existing diglycolamides.

Publications

Peer reviewed journals- published:

1. Jammu Ravi, K.A.Venkatesan, M.P.Antony, T.G. Srinivasan, P.R. Vasudeva Rao. Co-extraction and stripping behavior of trivalent actinides and fission products in *N,N*-di-2-ethylhexyl-*N',N'*-dioctyl-diglycolamide. *Radiochimica Acta*.101 (2013) 301-306.
2. Jammu Ravi, K. A. Venkatesan, M. P. Antony, T. G. Srinivasan, P. R. Vasudeva Rao. *J Radioanal Nucl Chem*. 295 (2013) 1283-1292. Tuning the diglycolamides for modifier-free minor actinide partitioning.
3. Jammu Ravi, T. Prathibha, K.A. Venkatesan, M.P. Antony, T.G. Srinivasan, P.R. Vasudeva Rao. *Sep. Purif. Technol.* 85 (2012) 96–100. Third phase formation of neodymium(III) and nitric acid in unsymmetrical *N,N*-di-2-ethylhexyl *N',N'*-dioctyldiglycolamide.
4. Jammu Ravi, A.S. Suneesh, T. Prathibha, K. A. Venkatesan, M. P. Antony, T.G.Srinivasan, P.R. Vasudeva Rao. *Solvent Extr. Ion Exch*, 29 (2011) 86–105. Extraction behavior of some actinides and fission products from nitric acid medium by a new unsymmetrical diglycolamide.
5. A.S. Suneesh, Jammu Ravi K.A. Venkatesan, M.P. Antony, T.G. Srinivasan, P.R. Vasudeva Rao. *J Radioanal Nucl Chem* 285 (2010) 653–658. Lanthanide-actinide separation by bis-2-ethylhexylphosphoric acid from citric acid-nitric acid medium.



Peer reviewed journals -Accepted:

6. Jammu Ravi, K.A. Venkatesan, M. P. Antony, T. G. Srinivasan, P.R. Vasudeva Rao. Unsymmetrical diglycolamide for the safe management of nuclear waste. (J. Environ. Chem. Eng. (2013), <http://dx.doi.org/10.1016/j.jece.2013.07.002> .
7. Jammu Ravi, B. Robert Selven, K. A.Venkatesan, M. P. Antony, T. G. Srinivasan, P.R. Vasudeva Rao. Evaluation of radiation stability of *N,N*-didodecyl *N',N'*-di-octyl diglycolamide- a promising reagent for actinide partitioning. (J.Radioanal.Nucl.Chem. DOI 10.1007/s10967-013-2776-4).
8. Jammu Ravi, B. Robert Selven, K. A.Venkatesan, M. P. Antony, T. G. Srinivasan, P.R. Vasudeva Rao. Radiolytic stability of di-2-ethylhexyl-dioctyl diglycolamide. (Accepted in Radiochimica Acta).

Peer reviewed journal papers under review:

9. Jammu Ravi, K. A.Venkatesan, M. P. Antony, T. G. Srinivasan, P.R. Vasudeva Rao, Evaluation of modifier-free di-dodecyl-di-octyl diglycolamide for partitioning of minor actinides from fast reactor high-level liquid waste.
10. Jammu Ravi, K. A.Venkatesan, M. P. Antony, T. G. Srinivasan, P.R. Vasudeva Rao. Development of a single-cycle method for partitioning of trivalent actinides using completely incinerable reagents from nitric acid medium.
11. Jammu Ravi, K.A.Venkatesan, M. P. Antony, T. G. Srinivasan, P.R. Vasudeva Rao. Unsymmetrical diglycolamides for the separation of trivalent actinides from nitric acid medium.

International conferences

1. Unsymmetrical diglycolamides for minor actinides partitioning.Jammu Ravi, K.A.Venkatesan, M.P.Antony, T.G. Srinivasan, P.R. Vasudeva Rao. Plutonium Futures- The Science 2012. Held at University of Cambridge, United Kingdom.(**Best presentation award**)
2. New usymmetrical diglycolamides for the extraction of americium(III) from nitric acid. Jammu Ravi, K.A.Venkatesan, M.P.Antony, T.G. Srinivasan, P.R. Vasudeva Rao. International Conference on Vistas in Chemistry (ICVC)-2011, p 140-141. Edt by V. Ganesan, S. Anthonysamy, Kitheri Joseph. Held at Indira Gandhi Centre for Atomic Research, Kalpakkam.

National symposia

1. Superior diglycolamides for minor actinide partitioning Jammu Ravi, K.A.Venkatesan, M.P.Antony, T.G. Srinivasan, P.R. Vasudeva Rao. In the Proceedings of Nuclear and Radiochemistry Symposium (NUCAR- 2013) held at Government Model Science College, R.D.University, Jabalpur, India, 2013.
2. Evaluation of unsymmetrical di-dodecyl-di-octyldiglycolamide for the separation of trivalent actinides from nitric acid medium valuation of didodecyl dioctyl diglycolamide for the partitioning of minor actinides.(**Best presentation award**) Jammu Ravi, K.A.Venkatesan, M.P.Antony, T.G. Srinivasan, P.R. Vasudeva Rao. In the Proceedings of Nuclear and Radiochemistry Symposium (NUCAR-2013), held at Government Model Science College, R.D.University, Jabalpur, India, 2013.
3. Radiolytic stability of *N,N*-di-2-ethylhexyl-*N',N'*-di-octyl-diglycolamideadiation stability of di-2-ethylhexyl-di-octyl diglycolamide. B. Robert Selvan, Jammu Ravi, K.A.Venkatesan, M.P.Antony,



- T.G. Srinivasan, P.R. Vasudeva Rao. In Proceedings of Nuclear and Radiochemistry Symposium (NUCAR- 2013), held at Government Model Science College, R.D.University, Jabalpur, India, 2013.
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 6. Extraction behaviour of fission products in di-2-ethylhexyl-di-octyl-diglycolamide from simulated high-level liquid waste.Jammu Ravi, K.A.Venkatesan, M.P.Antony, T.G. Srinivasan, P.R. Vasudeva Rao. In: Proceedings of DAE-BRNS Biennial Symposium on Emerging Trnends in Separation Science and Technology (SESTEC 2012). Edited by P.N. Pathak, R.M. Sawant, P.K. Mohapatra, A. Goswami, K.L. Ramakumar, Held at SVKM’s Mithibai college, Vile parle, Mumbai, India, 2012, p-89.
 7. Third phase formation of neodymium(III) in unsymmetrical diglycolamide. Jammu Ravi, T. Prathibha, K.A.Venkatesan, M.P.Antony, T.G. Srinivasan, P.R. Vasudeva Rao. In: Proceedings of Nuclear and Radiochemistry Symposium(NUCAR 2011). Edited by R.M. Sawant, S.K.Sali, Meera Venkatesh, V. Venugopal, Held at GITAM College, Visakapatnam, India, 2011, p-370.
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 9. Lanthanide-actinide separation by a modified TALSPEAK process. A.S. Suneesh, Jammu Ravi, K.A.Venkatesan, M.P.Antony, T.G. Srinivasan, P.R. Vasudeva Rao. In proceeding of BRNS Biennial Symposium on Emerging Trnends in Separation Science and Technology (SESTEC 2010). Edited by P.N. Pathak, R.M. Sawant, K.L. Ramakumar, V.K. Manchanda. Held at Indira Gandhi Centre for Atomic Research, Kalpakkam, India, 2010, p-403.



Name : **Karam Deo Shankhadhar**
Enrolment No. : MATH08200704001
Constituent Institute : Harish Chandra Research Institute, Allahabad
Title : On Certain Correspondences between Jacobi Forms and Modular Forms, and a Non-Vanishing Result for Half-Integral Weight L-Functions

Abstract

During my Ph. D., I worked on some problems related to modular forms and Jacobi forms. A brief description of the work is given below.

1. Restriction map for Jacobi forms (joint work with B. Ramakrishnan): In this work, we generalize the results of T. Arakawa and S. Bocherer for index 1 Jacobi forms (Abh. Math. Semin. Univ. Hambg. 69 (1999), 309-317; J. Reine Angew. Math. 559 (2003), 25-51) to higher index. We consider the index 2 case and show that the kernel of the restriction map is isomorphic to the certain space of vector-valued modular forms as well as isomorphic to a certain subspace of cusp forms and these two spaces are related with each other by a simple isomorphism. We obtain the injectivity of the direct sum of the first two differential operators on the space of weight 2 and index 2 Jacobi forms. We also obtain generalization of these results on certain subspace of Jacobi forms of square-free index.

2. Correspondence between Jacobi cusp forms and elliptic cusp forms (joint work with B. Ramakrishnan): In this work, we give a generalization of the correspondences obtained by K. Bringmann (Math Z. 253 (2006), 735-752), N. P. Skoruppa (J. Reine Angew. Math. 411 (1990), 66-95) and M. Manickam (Ph. D. thesis, 1989) to holomorphic and skew-holomorphic Jacobi cusp forms of matrix index and for congruence subgroups. As an application of our results, we obtain a correspondence between holomorphic (skew-holomorphic) Jacobi cusp forms of matrix index and holomorphic (skew-holomorphic) Jacobi cusp forms of integer index. In this work, the mappings involved in any correspondence are adjoint with respect to the Petersson scalar products.

3. Non-Vanishing of half-integral weight L-functions (joint work with B. Ramakrishnan): In 1997, W. Kohnen (J. Number Theory 67(1997), 182-189) proved certain non-vanishing result for L-functions associated to integral weight Hecke eigenforms. In this work, we extend Kohnen's method to the forms of half-integral weight. As a consequence of this result, we show that for any given point inside the critical strip, there exists a Hecke eigen cusp form of half-integral weight such that the corresponding L-function value at the point is non-zero and its first Fourier coefficient is also non-zero. It should be noted that the normalization of Fourier coefficients of forms of half-integral weight is still an open question.

4. Sign changes of Fourier coefficients of elliptic cusp forms and exponents of generalized modular functions (joint work with J. Meher and G. K. Viswanadham): In the first part of this work, we give a lower bound on the number of sign changes in certain subsequences of the Fourier coefficients of Hecke eigen cusp forms in the interval $(x, 2x]$. The second part of this work is about the sign changes of the q -exponents of a certain class of generalized modular functions on the Hecke congruence subgroup. We give a quantitative result on the number of sign changes in the subsequence of q -exponents of certain kind of generalized modular function at primes in the interval $(x, 2x]$.



Publications

1. (with B. Ramakrishnan) *On the restriction map for Jacobi forms*, Abh. Math. Semin. Univ. Hambg., DOI 10.1007/s12188-013-0081-3 (online first).
2. (with B. Ramakrishnan) *On a correspondence between Jacobi cusp forms and elliptic cusp forms*, Int. J. Number Theory (IJNT) 9 (2013), 917-937.
3. (with B. Ramakrishnan) *Non-vanishing of L-functions associated to cusp forms of half-integral weight*, Oman Conference Proceedings (Springer) (Accepted for publication).

Publication that is not included in the thesis

1. (with J. Meher and G. K. Viswanadham) *A short note on sign changes*, Proc. Indian Acad. Sci. (Math. Sci.) 123 (2013), 315-320.



Name : **Rajeev Singh**
Enrolment No. : PHYS10200605009
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Order-Disorder Transitions and Spatio-Temporal Pattern Formation in Complex Systems

Abstract

The appearance of simple or complex ordered patterns is a phenomenon of central importance in dynamical systems as well as in statistical physics of far-from-equilibrium systems. Several examples of the emergence of simple, regular patterns in physical systems that occur through collective order-disorder transitions, e.g., the aligned orientation of spins in Ising-like systems, are well known. In the context of nonlinear dynamics, similar simple ordering behavior can be observed in the synchronization of coupled oscillators. However, more complex patterns have recently been seen to occur in various systems under different conditions, especially in heterogeneous media. In this thesis, we have investigated how such patterns can arise by considering several models of complex systems comprising large number of components interacting with each other via non-trivial connection topologies. Such complexity is ubiquitous in the natural world (especially in living systems) and their spatio-temporal dynamics can often have functionally critical consequences for biological organisms. Our work is aimed at contributing towards building a general theory for describing pattern formation and ordering in “complex” systems.

The models we consider are capable of exhibiting a variety of novel complex patterns and collective order, some of which may in fact have manifestations in real systems, such as the mammalian uterus. We present systematic investigations of the mechanisms resulting in the generation of such patterns, which is a challenging exercise because of the large number of interacting components involved and the complicated nature of the coupling. The emergence of various dynamical regimes have been characterized in terms of distinct non-equilibrium steady state properties for systems that span a range of different types of components (in terms of their intrinsic behavior) and their interactions. At the level of component dynamics, the temporal behavior ranges from threshold-activated dynamics with either discrete-state transitions (as in “Ising”-like spins) or continuous-state behavior (as in excitable elements described by FitzHugh-Nagumo like equations) to those which display relaxation oscillations or even passive response (with any perturbation to the state decaying exponentially to the resting value). On the other hand, the nature of the interactions in the systems we have investigated range from exchange interactions (as in a system of spins) to diffusive coupling (e.g., in a system of cells coupled by electrical gap junctions describing a piece of biological tissue) to effective synapse-like connections (as between different brain areas in the cortex).

We have first shown that coupling non-oscillating dynamical elements gives rise to spontaneous coherent oscillations which has relevance for understanding the sudden emergence of contractions in the uterus at late stages of pregnancy. Next, we have explored the emergence of spatio-temporal patterns in arrays of coupled relaxation oscillators that can be realized in chemical microfluidics experiments. We have subsequently studied how globally coupled oscillators can exhibit a wide variety of patterns by spontaneously breaking the permutation symmetry of the dynamical system. This has implications for describing the dynamics of brain networks at a mesoscopic level which is accessible through EEG or fMRI experiments. Following this we have extended the concept of “chimera” state, originally introduced for systems of oscillators, to discrete dynamical system, viz., a system of classical Ising spins. This opens up the possibility of experimentally realizing chimera state in a variety of physical systems. Finally, we have investigated the approach to structural balance in networks using a simple



model of link-adaptation dynamics that shows non-trivial relaxation properties. Our results show that convergence to the balanced state can take extremely long times under certain conditions, which can potentially explain why balance may be difficult to observe in biological networks. We conclude with a discussion of how our results may contribute towards a general theory of pattern formation in complex systems and indicate possible future directions of research.

Published:

1. Singh, R., Dasgupta, S. and Sinha, S. (2011). Chimera order in spin systems. EPL (Europhysics Letters), 95, 10004. Arxiv Preprint, 1011.5032.
2. Singh, R., Xu, J., Garnier, N., Pumir, A. and Sinha, S. (2012). Self-Organized Transition to Coherent Activity in Disordered Media. Physical Review Letters, 108, 068102. Arxiv Preprint, 1201.1116.
3. Singh, R. and Sinha, S. (2013). Spatiotemporal order, disorder, and propagating defects in homogeneous system of relaxation oscillators. physical Review E, 87, 012907. Arxiv Preprint, 1206.2896.
4. Xu, J., Singh, R., Garnier, N., Pumir, A. and Sinha, S. (2013). Large variability in dynamical transitions in biological systems with quenched disorder. New Journal of Physics, 15, 093046. Arxiv Preprint, 1212.3466.

Communicated:

1. Singh, R., Menon, S. N. and Sinha, S. (2013). Complex patterns arise through spontaneous symmetry breaking in dense homogeneous networks of neural oscillators. Arxiv Preprint, 1305.7093.
2. Singh, R., Dasgupta, S. and Sinha, S. (2013). Extreme variability in convergence to structural balance in frustrated dynamical systems. Arxiv Preprint, 1307.8018.



Name : **Inbasekar Karthik**
Enrolment No. : PHYS10200704001
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : Attractor Mechanism in Gauged Supergravity

Abstract

In this thesis, we study the microscopic and macroscopic aspects of black holes in string theory. In particular, we study the counting of twisted BPS states in CHL models and derive the degeneracy formula. In the macroscopic side we study the generalised attractors in gauged supergravity. Specifically, we generalise the attractor mechanism to five dimensional gauged supergravity and construct explicit examples of Bianchi attractors. We then check the stability of the Bianchi attractors under scalar fluctuations about the attractor value. The metrics whose symmetry group factorise as a direct product of two dimensional Lifshitz symmetry and any homogeneous symmetry group given by the Bianchi classification correspond to stable attractors in the theory.

Publications

Published :

1. Karthik Inbasekar and Prasanta K. Tripathy, *Generalized Attractors in Five Dimensional Gauged Supergravity*, **JHEP** **1209** (2012) 003, arXiv:1206.3887 [hep-th]

Communicated:

1. Karthik Inbasekar and Prasanta K. Tripathy, *Stability of Bianchi Attractors in gauged supergravity*, (to appear in **JHEP**) , arxiv: 1307.1314 [hep-th]

Preprints:

1. Karthik Inbasekar and Suresh Govindarajan, *A non-commuting twist in the partition function*, arxiv: 1201.1628 [hep-th]



Name : **Pampa Paul**
Enrolment No. : MATH10200704001
Constituent Institute : Institute of Mathematical Sciences, Chennai
Title : L0-Types Common to a Borel-DE Siebenthal Discrete Series and its Associated Holomorphic Discrete Series

Abstract

Let G_0 be a simply connected non-compact real simple Lie group with maximal compact subgroup K_0 . Let $T_0 \subset K_0$ be a maximal torus. Assume that $\text{rank}(G_0) = \text{rank}(K_0)$ so that G_0 has discrete series representations. We denote \mathfrak{g} , \mathfrak{l} and \mathfrak{t} by and the complexifications of the Lie algebras \mathfrak{g}_0 , \mathfrak{k}_0 and \mathfrak{t}_0 of G_0 , K_0 and T_0 respectively. Denote by Δ the root system of \mathfrak{g} with respect to \mathfrak{t} . There exists a positive root system known as the Borel-de Siebenthal positive system such that there is exactly one non-compact simple root, denoted ν . We assume that G_0/K_0 is not Hermitian. In this case one has a partition $\Delta = \cup_{-2 \leq i \leq 2} \Delta_i$ where $\alpha \in \Delta$ belongs to Δ_i precisely when the coefficient of ν in α when expressed as a sum of simple roots is equal to i . Let G be the simply connected complexification of G_0 . Denote by L_0 and \bar{L}_0 , the centralizer in K_0 of a certain circle subgroup S_0 of T_0 and its image in G (under the homomorphism $\rho : G_0 \rightarrow G$ defined by the inclusion $\mathfrak{g}_0 \rightarrow \mathfrak{g}$) respectively so that the root system of (L_0, T_0) is Δ_0 . Any \bar{L}_0 -representation is regarded as an L_0 -representation via ρ .

Let γ be the highest weight of an irreducible representation of \bar{L}_0 such that $\gamma + \rho_{\mathfrak{g}}$ is negative on $\Delta_1 \cup 2$. Here $\rho_{\mathfrak{g}}$ denotes half the sum of positive roots of \mathfrak{g} . Then $\gamma + \rho_{\mathfrak{g}}$ is the Harish-Chandra parameter of a discrete series representation $\pi_{\gamma + \rho_{\mathfrak{g}}}$ of G_0 called a Borel-de Siebenthal discrete series representation. The K_0 -finite part of $\pi_{\gamma + \rho_{\mathfrak{g}}}$ is admissible for a simple factor $K_1 \subset K_0$. It turns out that $S_0 \subset K_1$ and $K_1/L_1 = K_0/L_0$ is a Hermitian symmetric space where $L_1 = L_0 \cap K_1$. One has a Hermitian symmetric pair of non-compact type (K_1^*, \bar{L}_0) dual to the pair (K_0, L_0) . The element γ also determines a holomorphic discrete series representation $\pi_{\gamma + \rho_{\mathfrak{g}}}$ of K_1^* .

In my thesis the following question is addressed : Does there exist common L0-types between the Borel-de Siebenthal discrete series representation $\pi_{\gamma + \rho_{\mathfrak{g}}}$ and the holomorphic discrete series representation $\pi_{\gamma + \rho_{\mathfrak{g}}}$? We settle this question completely in the quaternionic case, namely, when $L_1 \cong su(2)$. In the general case, affirmative answer is obtained under the following two hypotheses—(i) there exists a (non-constant) relative invariant for the prehomogeneous space $(L_0^C; u_1)$, where u_1 is the representation of L_0 on the normal space at the identity coset for the (holomorphic) imbedding $K_0/L_0 \rightarrow G_0/L_0$, and, (ii) the longest element w_1^0 of the Weyl group of K_0 normalizes L_0 . The proof uses, among others, a decomposition theorem of Schmid and Littelmann’s path model.

Publications

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Title : Structure Phase and Formation of Novel Phases Involving Intra-Group IV Elements at High P-T Conditions

Abstract

Phase transformations in materials can occur either by varying temperature or pressure or both simultaneously. This thesis illustrates the fascinating role that simultaneous application of pressure and temperature can play in inducing chemical bond formation between seemingly unreactive elements belonging to Group IV of the periodic table. Investigations of IV-IV systems in bulk or thin film forms, have attracted widespread attention from both basic and technological view points. The bulk synthesis is unsuccessful using conventional methods due to their low solubility and large ionic radii differences, structures, etc at ambient P-T conditions. A novel idea has been attempted in this thesis to overcome these: By subjecting a mixture of the two group IV elements to pressures close to a structural transition pressure of one of them and simultaneously heating the mixture using high power IR lasers these differences can be minimized and new bond formation may occur. Laser heated diamond cell experiments carried out first on binary mixtures of group-IV elements, Ge and Sn, at ~ 7.6 GPa and ~ 2000 K, indeed reveal two new Raman modes that could unambiguously be attributed to new Ge-Sn bonds formed at high P-T conditions, when the Ge phase is at the verge of structural instability. Persistence of these modes down to atmospheric pressure indicates the stable nature of the bonds. This prescription of inducing novel bond formation at high P-T conditions could be further validated in the case of Ge-C system.

The other class of investigations presented in the thesis pertains to studying interesting pressure induced structural behavior shown by lead containing matlockite systems, PbFCl and PbFBr. Of these, PbFCl is a prototype for the matlockite structure compounds and crystallize in tetragonal structure with space group $P4/nmm$. High pressure X-ray diffraction studies (HPXRD) and Raman spectroscopy have been carried out on PbFCl for the first time. Pressure dependence of various inter- and intra- layer Raman modes were studied up to ~ 41 GPa. The low-frequency interlayer vibrational modes, $A_{1g}(1)$ and $E_g(1)$, identified as rigid-layer modes, exhibit non-monotonic behavior with increasing pressure. They exhibit points of inflexion at ~ 24 GPa and ~ 31 GPa respectively, indicating onset of a subtle instability. Emergence of a new Raman mode at ~ 24 GPa and a large increase in the intensity of the $A_{1g}(1)$ mode signify occurrence of a symmetry lowering structural transition of the parent tetragonal phase with enhanced interlayer coupling. Two more modes appear at higher pressures (~ 33 GPa) at frequencies below the $A_{1g}(1)$ mode and are ascribed to a distorted phase (monoclinic). HPXRD studies performed up to ~ 47 GPa confirm the occurrence of the structural transitions with decreasing crystal symmetry. Similar behavior is shown by the homologous compound, PbFBr. These observations have been rationalized by a mechanism in which structural distortions involves destabilization of the tetragonal unit cell following a gradual change in the bonding nature from layer-like (2D) to non-layer like (3D) involving the Cl- bi-layers along the c direction.

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4. N. Subramanian and Y.A. Sorb, *Pressure Induced Structural Changes in BaFCl and PbFCl: A Comparison*, 24th Annual General Meeting of Materials Research Society of India (MRSI) Kalpakkam, India P.41 (2013)
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Title : Studies on Thin Films of Zr, ZrN and ZrAlN Prepared by Pulsed Magnetron Sputtering : Microstructures, Thermal Expansion, Nanomechanical and Tribological Properties

Abstract

ZrN based hard coatings are of great interest in a number of technological applications due to their improved tribological, corrosion, mechanical and physical properties. Also, the addition of Al to ZrN has been reported to progressively modify the texture, improve the resistance against oxidation and also increase significantly the hardness of the films. In the present work, a systematic investigation is reported on the structural and nanomechanical properties of thin films of Zr, ZrN and alloyed ZrAlN deposited on (100) Si and D-9 alloy substrates by pulsed DC magnetron sputtering as a function of substrate temperature and nitrogen partial pressure. A study has been undertaken to investigate the thermal stability and thermal expansion behavior of these thin films. Also, the inter-relationship between microstructures, nanomechanical, and tribological properties of these films is investigated.

Formation of α -phase of zirconium with [001] preferred orientation was noticed in the temperature range 300–873 K. It was found that crystallite size increased with increasing temperature. Nanoindentation and microhardness measurements of Zr films showed that the hardness of the films was in the range 6–10 GPa. Scratch test results indicated that the films deposited at higher substrate temperature have better adhesion. High temperature x-ray diffraction showed that Zr films were stable up to 773 K.

The effect of substrate temperature and nitrogen flow rate on the growth characteristics, nanomechanical and tribological properties and phase stability of ZrN films were studied. Only fcc-ZrN was obtained by reactive sputtering at lower flow rates of nitrogen (< 2sccm). At higher flow rates of nitrogen (\geq 2sccm), small amounts of orthorhombic-Zr₃N₄ phase was formed along with ZrN. TEM studies also confirmed the presence of ZrN along with small higherflow rates of nitrogen (\geq 2sccm), small amounts of orthorhombic-Zr₃N₄ phase was formed along with ZrN. TEM studies also confirmed the presence of ZrN along with small amount of Zr₃N₄ phase at higher nitrogen flow rates. HTXRD study showed that ZrN films were stable up to 1073 K. Nanomechanical properties of ZrN films showed peak values of hardness (H) and elastic modulus (E) for the films deposited at 1-2 sccm flow rate of nitrogen. The effect of nitrogen flow rate on the nanomechanical properties indicated an enhancement in hardness and elastic modulus and showed a peak value for the resistance to plastic deformation (H₃/E₂) at lower flow rates of nitrogen. The tribological properties of ZrN thin films were found to be influenced by the deposition temperature and sliding counter bodies.

Zr_{1-x}Al_xN_y films have been studied with the Al concentration range of $0 \leq x \leq 0.36$ Al and it was found that (Zr,Al)N was in solid solution up to 36 at. % of Al. Alloyed films of ZrAlN exhibited a fcc structure. As the Al content was increased up to 36 at.%, lattice parameter decreased due to the substitution of Zr by Al of lower atomic radius. HTXRD results of Zr_{1-x}Al_xN_y thin films indicated that the addition of Al improved the phase stability at higher temperature in comparison with ZrN. The average linear thermal expansion coefficient of Zr_{1-x}Al_xN_y thin films showed increase in the thermal expansion coefficient with increasing Al content up to 28 at.%Al. It was also observed that values of hardness and Young's modulus of the



alloyed ZrAlN films were in the range of 9-18 GPa and 235-365 GPa, respectively. Tribological studies of ZrAlN thin film showed that the COF of alloyed films of ZrAlN was lower for the steel ball (100Cr6 steel) than that for the Al₂O₃ ball up to 36 at. % of Al. However, no clear trend in the COF was noticed as a function of Al addition. The variations in the nanomechanical and tribological properties have been discussed in relation with the microstructures of these films. $\frac{3}{2}$ at lower flow rates of nitrogen. The tribological properties of ZrN thin films were found to be influenced by the deposition temperature and sliding counterbodies. Zr_{1-x}Al_xN_y films have been studied with the Al concentration range of $0 \leq x \leq 0.36$ Al and it was found that (Zr,Al)N was in solid solution up to 36 at. % of Al. Alloyed films of ZrAlN exhibited fcc structure. As the Al content was increased up to 36 at. %, lattice parameter decreased due to the substitution of Zr by Al of lower atomic radius. HTXRD results of Zr_{1-x}Al_xN_y thin films indicated that the addition of Al improved the phase stability at higher temperature in comparison with ZrN. The average linear thermal expansion coefficient of Zr_{1-x}Al_xN_y thin films showed increase in the thermal expansion coefficient with increasing Al content up to 28 at. % Al. It was also observed that values of hardness and Young modulus of the alloyed ZrAlN films were in the range of 9-18 GPa and 235-365 GPa, respectively. Tribological studies of ZrAlN thin film showed that the COF of alloyed films of ZrAlN was lower for the steel ball (100Cr6 steel) than that for the Al₂O₃ ball up to 36 at. % of Al. However, no clear trend in the COF was noticed as a function of Al addition. The variations in the nanomechanical and tribological properties have been discussed in relation with the microstructures of these films.

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6. Studies of microstructural and nanomechanical properties of ZrAlN thin films prepared by pulsed magnetron sputtering. Akash Singh, P. Kuppasami, R. Thirumugesan, R. Ramaseshan, E. Mohandas and S. Das (to be communicated to Surface and Coatings Technology).
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Title : Studies on Thin Films of Zr, ZrN and ZrAlN Prepared by Pulsed Parameterized Graph Separation Problems: New Techniques and Algorithms

Abstract

Menger's theorem, which states that the minimum number of vertices whose removal disconnects two vertices s and t in a graph is equal to the maximum number of pairwise vertex disjoint paths from s to t in the graph, is an extremely fundamental theorem in combinatorial optimization and it is known that the minimum s - t cut can be computed in polynomial time. Generalizations of the problem of finding the minimum set of vertices in graph, are called *graph separation problems*. The main problems we study in this thesis are such graph separation problems. The fact that very natural generalizations of the s - t cut problem turn out to be NP- complete has motivated the study of these problems in the framework of Parameterized Complexity and the study of these problems has even emerged as an extremely active and independent subfield over the last few years.

In the Parameterized Complexity framework, for decision problems with input size n , and a parameter k , the goal is to design an algorithm with runtime $f(k) n^{O(1)}$ where f is an arbitrary function of k , as opposed to (in most cases,) a trivial $n^{k+O(1)}$ algorithm. Such algorithms are called fixed parameter tractable (FPT) and problems with FPT algorithms are said to be fixed parameter tractable (FPT).

The reasons behind the recent flurry of activity with respect to graph separation problems are twofold. Firstly, these problems themselves present independent challenging combinatorial questions. Secondly, a lot of classical problems which are not graph separation problems or even graph problems in some cases, have been found to have a graph separation problem at their core. Notable examples of this include the VERTEX COVER problem, the ALMOST 2-SAT problem, DELETION q-HORN BACKDOOR SET DETECTION, and SATISFIABILITY. Such frequent occurrences of graph separation problems at the heart of various seemingly unrelated problems has also contributed towards the interest in this direction. In this thesis, we

- design new techniques and frameworks to obtain new as well as improved FPT algorithms for certain kinds of parameterized graph separation problems;
- present problems which are not graph separation problems themselves, but have some variant of graph separation at their core, after which by using our new frameworks as well as existing ones, we give new as well as improved FPT algorithms.

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Name : **Ajay Kumar Mishra**
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Title : High Pressure Investigations on Some Geophysically Relevant Materials Geophysically Relevant Materials

Abstract

The thesis unravels the high pressure phenomenon studied on geophysically relevant materials encompassing a wide range of substances from zircon and scheelite structured family, pyrochlores, perovskites and phosphate materials using x-ray diffraction and Raman scattering techniques. These measurements help to understand the detailed structural as well as vibrational behaviour of the materials at atomic scale.

In this thesis, the first chapter deals with the introduction to high pressure physics followed by crystallography and phase stability under high pressure. The latter part of this chapter describes the x-ray diffraction, Raman scattering and high pressure generation techniques especially the diamond anvil cell which makes it possible to perform in-situ measurements under high pressure. The next four chapters of this thesis describe the structural behaviour of the geophysically relevant materials. In one of the studies on zircon structured nano crystalline chromates (YCrO_4 and HoCrO_4), it has been shown that zircon to scheelite transformation takes place through an intermediate monoclinic phase which has been stabilized and observed in these compounds. The phase transition pressure (zircon to scheelite) is higher than that in bulk chromates. The compression of scheelite structured LiErF_4 leads to pressure induced amorphization at ~ 28 GPa preceded by two structural phase transitions. Softening of E_g mode and absence of discontinuous change in volume drop implies the scheelite to fergusonite phase transition to be second order in nature. The c/a ratio of fluoroscheelite compounds increase with pressure in contrast to oxyscheelite compounds where it decreases with pressure. These studies also indicate that the high pressure behavior of LiErF_4 does lie in between the end members LiYF_4 and LiGdF_4 .

Pressure can lead to order disorder kind of transition is exemplified by the high pressure studies on pyrochlore compounds ($\text{Yb}_2\text{Ti}_2\text{O}_7$ and $\text{Dy}_2\text{Ti}_2\text{O}_7$). The x-ray diffraction and Raman scattering measurements on $\text{Yb}_2\text{Ti}_2\text{O}_7$ show that it undergoes a first order structural phase transition from cubic to a monoclinic phase ($P2_1/c$) which has cation occupancy disorder. At further higher pressures the anionic disorder in the oxygen lattice appears. The P-V behavior of $\text{Dy}_2\text{Ti}_2\text{O}_7$ shows a subtle structural distortion across ~ 9 GPa with a possible lattice distortion at this pressure. The anionic lattice disorder is evident in this compound at high pressures.

The high pressure studies on perovskite materials are important from geophysical point of view. The synchrotron based ADXRD studies on rhombohedrally distorted multiferroic perovskite BiFeO_3 shows that it undergoes two structural phase transition, both to orthorhombic symmetry in contrast to earlier studies where its intermediate phase was having monoclinic symmetry. The other two perovskites BaLiF_3 and Sr_2MgWO_6 are structurally stable up to half a mega bar pressures. The studies on uranium phosphate show that compression can stabilize the uranium in two valencies in this compound. The last chapter describes the development of EDXRD beam line suitable for studies under constrained geometry.



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16. Structural Phase Transitions in LiErF_4 _A.K.Mishra, Nandini Garg, A.K.Tyagi and Surinder M. Sharma To be communicated to Phys. Rev. B



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Title : Positron Annihilation of Model Fe-Cr Alloys and Ferritic/Martensitic Steels

Abstract

Positron annihilation spectroscopy studies are carried on Ferritic/Martensitic (F/M) steels and Fe-Cr binary alloys. The present thesis work on F/M steels is aimed at bringing out the correlation between positron annihilation characteristics and microstructural changes due to different thermo-mechanical treatments. Work on Fe-Cr binary alloys is aimed at understanding non-equilibrium conditions which segregate Cr locally, temperature range at which they are stable and the nature of the phases formed due to Cr segregation. This thesis also presents the design of a special geometry for Doppler broadening based NDT positron system and a methodology to find out the signal to background ratio. Preliminary test results are reported.

Positron annihilation studies on F/M steels showed that positron annihilation characteristics are sensitive to the microstructural changes such as the nucleation, growth and coarsening of precipitates and martensitic phase formation. They also demonstrated a unique sensitivity to annealing of open volume atomistic defects as compared to other techniques such as ultrasonic velocity, hardness and XRD. Further, the growth and coarsening stages can be distinguished using positron lifetime. The correlation between positron lifetime, ultrasonic velocity and hardness is found to be useful to distinguish distinct microstructures induced by thermal treatments.

Studies in Fe-9Cr alloys have shown that dislocations play a major role in accelerating Cr segregation. Initial microstructure of the alloy is found to have considerable influence on Cr segregation. Isothermal studies have revealed that Cr precipitates are formed at temperature as low as 723 K and they are found to be unstable above 873 K. In Fe-15Cr and Fe-20Cr alloys, with no prior dislocations, it is understood that at 748 K α' -phase forms and subsequent treatment at 873 K converts this into intermetallic σ -phase. By analogy and selected area diffraction patterns, the segregated phase formed in Fe-9Cr alloys is also ascertained to be σ -phase.

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9. On the nature of Cr segregation in Fe-Cr alloys: A positron annihilation studym S. Hari Babu et.al. (manuscript under preparation)

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Name : **Varghese Anto Chirayath**
Enrolment No. : PHYS02200704014
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Study of Near Surface Defects Using Positrons and Development of a Pulsed Positron Beam System

Abstract

Positron annihilation spectroscopy with low energy positrons has been utilized to investigate the defect structure and their thermal evolution in two model systems viz., n-type Cz-Silicon (100) and highly oriented pyrolytic Graphite (HOPG).

Defects are created in Cz Si (100) through nitrogen ion implantation at two doses - 10^{14} and 10^{15} ions/cm². Isothermal evolution studies using slow positron beam revealed the existence of trans-projected range defects and their annealing by 473 K in the high dose sample. Nitrogen – Vacancy complex formation is detected in low dose sample at 873 K using the S-W correlation plot and the variation of W parameter with positron energy. The existence of such complexes is not visible in high dose sample, where the segregation of open volume defects near surface dominates the S-parameter and W-parameter signals for 873 K. Secondary ion mass spectroscopy (SIMS) revealed anomalous surface diffusion of nitrogen for high dose sample at 1073K and the dependence of oxygen in-diffusion on the presence of Nitrogen.

Defects are created in HOPG using controlled self ion implantation at 10^{14} and 10^{15} ions/cm². Using Atom Force Microscopy (AFM), Raman spectroscopy and slow positron beam spectroscopy a comprehensive picture on damage evolution in graphite is presented. Studies revealed a fast annealing process corresponding to interstitial vacancy recombination and a slow process related to vacancy migration towards the surface. Both processes depend on the density of the defects present, as observed in the low dose and high dose samples. Existence of a defect species, which is stable upto 673 K is detected in high dose sample, which is predicted to be interlayer divacancy. Vacancy migration along the c-axis is seen in both the samples at temperatures much lower than the predicted migration barriers.

To improve the ability to detect the nature and concentration of defects in a depth resolved manner, a pulsed positron beam based lifetime system is designed in the second part of the thesis. The working of the beam pulsing system is simulated and important process parameters like the amplitudes of the modulation voltages and their phases are derived. Based on these design considerations, an ultra high vacuum system, the magnetic beam guidance, 1200 velocity filter, the pulsing electrodes and the acceleration systems were fabricated. The extraction and transport of slow positrons through the assembled system is achieved and depth specific S parameter measurements are demonstrated for two standard samples. The electrical connection to the pulsing electrodes in the vacuum side is completed and has been incorporated into the beam line for the integration of RF power to the pulsing system and for the final testing of the lifetime system.

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2. Anto C V, Arunkumar J, Rajaraman R, Nair K G M and Amarendra G 2011 "Characterization of Vacancy Defects in Carbon Ion Irradiated Graphite Using Positrons" AIP Conf. Proc. 1349, 1281.
3. Anto C V, Rajaraman R, Abhaya S, Parimala J and Amarendra G 2011 "Design optimization of a pulsed positron beam system at IGCAR, Kalpakkam" J. Phys.: Conf. Ser. 262 012062.
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8. Ragunathan V, Hari Babu S, Anto C V, Rajaraman R, Amarendra G, Saroja S, Sundar C S, Ana Alamo and Baldev Raj 2009 "Positron annihilation studies on 9Cr Reduced Activation Ferritic/Martensitic steels" Physica Status Solidi (c) 6 2307. *

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To be submitted/under preparation

1. Anto C V et. al. 2013 "Defect evolution in Carbon ion implanted Highly Oriented Pyrolytic Graphite: Positron and Raman Spectroscopic studies"
2. Anto C V et.al. 2013 "Slow Positron beam extraction and design of a pulsed positron beam"
3. Anto C V et.al. 2013 "Development of a beam based lifetime system"
4. Anto C V et.al. 2013 "Ligament coarsening in Nanoporous Gold : A positron Annihilation Study" *

* Not included in thesis



Name : **Sijoy C.D.**
Enrolment No. : PHYS01200804008
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Physics of Magnetic Flux Compression Using Plasma Armatures
Using Finite Difference Time Domain Method

Abstract

Various schemes have been analysed over the years for extracting energy from Inertial Fusion Energy systems such as laser-driven fusion. The method examined here is to directly convert a part of the plasma kinetic energy into pulsed electrical energy, through the medium of magnetic flux compression. The present work involves a computational study of the physics of flux compression inside a current-carrying coil by an expanding inertial fusion plasma sphere. The numerical analysis has been performed using two-dimensional MHD and FDTD simulations.

The overall efficiency of the system is determined numerically for a typical set of initial plasma and system parameters. It is found that the proposed system is promising in terms of overall efficiency, but the system produces ultrahigh inter-turn voltages in the coil, necessitating the use of magnetic self-insulation to avoid inter-turn breakdown.

The plasma sphere, expanding across a magnetic field, is subject to the Magnetic Rayleigh-Taylor (MRT) instability. For a detailed analysis of this concept, especially plasma dynamics under large deformations, a two-dimensional Eulerian multi-material MHD model has been developed for the first time. The algorithm is found to be capable of accurately handling complex plasma dynamics inside the MFC system. Magnetic field diffusion into the plasma during the expansion phase is found to be negligible. 2D MHD simulations of random, single and multi-mode MRT instability growth have been performed to analyze the MRT instability and its implications for the proposed MFC system. The simulation takes into account the effects of MFC and geometric divergence due to spherical plasma expansion.

The dominant modes obtained in the random seed analysis show a progressive transition to the intermediate wavelength regime ($\sim 4-8$ cm) in the spectrum. Single-mode evolution exhibits linear exponential growth followed by a non-linear phase towards stagnation time. In the multi-mode analysis, with initial amplitudes (α_{in}) comparable to the perturbation wavelength (λ_{in}), there is clear evidence of mode coupling and the generation of harmonic and inverse cascade modes. We also find that near the time of stagnation, the growth in amplitude of the modes, although exponential in nature, is much lower than that predicted by linear theory. Furthermore, the instability amplitudes are not large enough for $\alpha_{in} \leq 0.1 \lambda_{in}$ to severely disturb the smooth MFC during the first expansion phase. However, the growth of modes with $\alpha_{in} \geq \lambda_{in}$ causes plasma jetting, especially for longer λ modes, and can lead to significant reduction in MFC efficiency.

We have also investigated the application of finite difference time domain (FDTD) schemes, involving direct solution of Maxwell's equations. The FDTD algorithm has been modified, for the first time, by including motional e.m.f terms in the standard FDTD update equations. This algorithm can be applied to MFC systems with moving parts. This new approach is validated with standard analytical solutions for planar flux compression systems and magnetic field diffusion in moving conductors with non-relativistic velocity. Finally, in order to demonstrate the utility of this powerful scheme to MFC problems, we have applied it to a sample problem involving plasma armatures. To our knowledge, this is the first application of this powerful technique to such systems. We have also identified, through extensive



numerical tests, critical constraints that must be satisfied while performing magnetic diffusion problems using FDTD scheme.

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2. An Eulerian MHD model for the analysis of magnetic flux compression by expanding diamagnetic plasma sphere, Sijoy C. D. and S. Chaturvedi, *Fusion Engineering and Design*, 87, pp 104- 117, (2012).
3. Conversion of plasma energy into electrical pulse by magnetic flux compression, Sijoy C. D. and S. Chaturvedi, *Fusion Engineering and Design*, 86, pp 174- 182, (2011).
4. Volume of fluid algorithm with different modified dynamic material ordering methods and their comparison, Sijoy C. D. and S. Chaturvedi, *Journal of Computational Physics*, 229, pp 3848-3863, (2010)
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6. Calculation of Accurate Resistance and Inductance for Complex Magnetic Coils using the Finite Difference Time Domain Technique, Sijoy C. D. and S. Chaturvedi, *IEEE Transactions on Plasma Science*, 36, pp 70-79, (2008).
7. A VOF based multi material method to study impact and penetration problems, Sijoy C. D., V. Mehra, V. Mishra and S. Chaturvedi, *Journal of Physics Conference Series*, 377, pp 012106, (2012)

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2. Three Dimensional Calculations of Electrical Parameters in Flux compression Systems, Sijoy C. D. and S. Chaturvedi, Proc. 2006 International Conference on Megagauss Magnetic Field Generation and Related Topics, Santa Fe, New Mexico, USA, pp 385-390 (2006).
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6. Sijoy C. D., V. Mehra, V. Mishra and S. Chaturvedi, 23rd International Conference on High Pressure Science and Technology (AIRAPT), Mumbai, (2011)
7. Rayleigh-Taylor instability analysis in a direct energy conversion system based on magnetic flux compression by expanding fusion plasma, Sijoy C. D., G. Singh and S. Chaturvedi, 27th National Symposium on Plasma Science and Technology, University of Pondichery, Pondichery, Dec. (2012).



Name : **Ambresh Kumar Shivaji**
Enrolment No. : PHYS07200604037
Constituent Institute : Institute of Physics, Bhubenswar
Title : Gluon Fusion Processes at One-Loop within the Standard Model and Beyond

Abstract

Due to a large gluon luminosity available at the Large Hadron Collider (LHC), the gluon fusion processes play an important role in our quest for new physics, beyond the well established laws of the standard model of particle physics. In this thesis, we have studied certain gluon fusion processes which proceed via quark loop diagrams at the leading order. The fact that these gluon-gluon channel processes are independent processes, their contributions towards the total/differential hadronic cross sections can be calculated separately. One of the most important part of such calculations involves the reduction of one-loop tensor integrals into a suitable set of one-loop scalar integrals. We have extended the existing codes and have developed new codes for this purpose.

We have considered the production of a pair of electroweak bosons in association with a jet via gluon fusion within the standard model. These processes were not accessible at earlier hadron colliders such as the Tevatron. Therefore, observation of these rare processes at the LHC will be a test of the standard model itself. Like the vector boson production via gluon fusion processes, these processes are also important backgrounds for many new physics signals and the standard model Higgs boson signal at the LHC. These leading order gluon fusion processes contribute to the corresponding hadronic processes at the next-to-next-to-leading order in the strong coupling parameter (α_s). We have reconfirmed the importance of $g g \rightarrow \gamma \gamma j$ process at the LHC. We find that its cross section at the 8 TeV center-of-mass energy is about 0.78 pb. We have performed a comparative study of $g g \rightarrow \gamma Z$, $g g \rightarrow Z Z j$, and of $g g \rightarrow W^+ W^- j$ processes and find that their contributions towards total hadronic cross sections is in the range of 4-15 % as compared to the corresponding tree-level contributions. The percentage contributions increase as we go to higher collider center-of-mass energies. In a more complete study of $g g \rightarrow \gamma Z j$ process, we have also presented various phenomenologically important kinematic distributions at 8 TeV LHC. The dependence of our results on the choice of parton distribution function sets and on the choice of scales are also studied. Calculation of multi-particle one-loop processes often suffer from the issue of numerical instability near exceptional phase space points. Various strategies that we have adopted to deal with this problem, are also discussed.

We have taken a model of extra-dimensions, the ADD (Arkani-Hamed, Dimopoulos and Dvali) model, as the possible candidate of new physics at the LHC. This model tries to solve the hierarchy problem of the standard model by proposing large extra space dimensions which may be accessible at TeV scale. We have considered the direct production of KK-gravitons (G_{kk}) in association with an electroweak boson ($H/\gamma/Z$) via gluon fusion. These processes contribute to the corresponding hadronic processes at the next-to-leading order in α_s . We have presented results for 14 TeV LHC. Due to the charge-conjugation properties of various fields, we find that the $g g \rightarrow \gamma G_{kk}$ amplitude vanishes at the leading order. We observe a significant cancellation in both $g g \rightarrow H G_{kk}$ and $g g \rightarrow Z G_{kk}$ amplitudes, leading to smaller cross sections, of the order of few fb at 14 TeV. In $g g \rightarrow Z G_{kk}$ case, we have come across linearly divergent box diagrams which like the VVA triangle diagrams, give rise to anomaly. We have studied systematically the dependence of our results on various model parameters. The scale dependence and the choice of parton distribution function sets are also discussed.



These gluon fusion processes also provide a great opportunity to understand many special properties of fermion loop amplitudes. We have proved that the most general fermion loop *diagram* is always infrared finite. We observe that the rational part of a ultra-violet (UV) finite fermion loop diagram is independent of the masses of internal lines. This allows one to extract the complete rational part of UV finite fermion loop amplitude in the infinite fermion mass limit. We have verified these properties in all our processes considered in the thesis.

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5. Di-Vector Boson + Jet Production via Gluon Fusion at Hadron Colliders, P.Agrawal and A.Shivaji, arXiv:1207.2927 [hep-ph].
6. Production of $\gamma Z g$ and associated processes via gluon fusion at hadron colliders, P.Agrawal and A.Shivaji, arXiv:1208.2593 [hep-ph].



Name : **Manoj Mohapatra**
Enrolment No. : CHEM01200604018
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Spectroscopic Investigation of Radiation Induced Effects in Borosilicate Glasses used for Immobilization of Nuclear Wastes

Abstract

Borosilicate based glass formulations have been now widely accepted as the matrix for fixing the high level radioactive liquid waste (HLW) generated after the reprocessing of the spent nuclear fuel. However, the exact composition of the glass depends on the composition of the HLW, which in turn depends on the type of reactor, burn up, off reactor cooling of spent nuclear fuel and nature of reprocessing flow sheets etc. At Bhabha Atomic Research Centre (BARC), Trombay, the historic waste from the research reactors is characterized by the presence of high amounts of sulphate ions coming from the ferrous sulphamate used for reducing Pu(IV) to Pu(III). For the sulfate rich HLW, a barium oxide containing alkali borosilicate glass was developed and is routinely used for the waste vitrification. Because of the radioactive components present in the HLW, the glass experiences radiation damage. Spectroscopic techniques provide non-invasive and direct method for characterizing these radiation induced changes in the glass samples.

In the present doctoral thesis submitted to Homi Bhabha National Institute (HBNI), Mumbai, extensive work has been carried out to understand the radiation effects in Trombay nuclear waste glasses, using conventional photon based techniques, such as photoluminescence spectroscopy (PL), Photoacoustic Spectroscopy, FTIR (Fourier Transform Infra Red) and Raman. Also novel techniques like positron annihilation spectroscopy (PAS) and Electron Spin Resonance (ESR) spectroscopy were used to understand the radiation induced changes in the glass matrix.

ESR can give information regarding the chemical nature of defect centers formed in the irradiated glass and quantify them. On the other hand, FTIR and Raman spectroscopy can give information about the changes in the bulk glass network.

The glasses were irradiated with gamma rays, electron beam and heavy ions to get an overall idea regarding the radiation induced changes in the system. From these experiments it was inferred that the borosilicate glass samples used for nuclear waste vitrification, undergo a lot of structural modification on irradiation by energetic radiations.

However, the overall glass network remains unaffected to a large extent by the irradiation. This is in agreement with the overall IR and Raman data that showed only marginal changes in the irradiated samples. It is worth mentioning here that all the above results have been performed with high dose rate (because of high ion beam /electron current) which can cause some effects that might not actually occur in the HLW glasses irradiated at the same total dose. However, the nature of radiation

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1. EPR investigations of electron beam irradiated Trombay waste base glass, **M.Mohapatra**, R.M.Kadam, B.S.Tomar, R.K.Mishra, C.P.Kaushik, S.V.Godbole, K.Raj and V.K.Manchanda, *IOP Conf. Series: Materials Science and Engineering 2* (2009) 012022
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- Tomar, Kanwar Raj, S. V. Godbole & V. K. Manchanda, *Physics and Chemistry of Glasses* 51 (2010) 217
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2. Photoacoustic spectroscopic and electron paramagnetic resonance investigations on copper doped alkali borosilicate glasses, A R Dhobale, **M. Mohapatra**, R M Kadam, Mithlesh Kumar, C P Kaushik and S V Godbole, *IOP Conf. Series: Materials Science and Engineering* 2 (2009) 012044
3. Photoluminescence and photoacoustic investigations of U and Th in nuclear waste glass, A.R.Dhobale, **M. Mohapatra**, R.K.Mishra, C.P.Kaushik and S.V.Godbole, *International Journal of Applied Glass Science* 1 (2010) 322

Symposium / Conference Publications

1. EPR and PL investigation of Cr incorporated barium borosilicate Glass, R.M.Kadam, **M. Mohapatra**, B.S.Tomar, R.K.Mishra, S.N.Tripathy, C.P.Kaushik, S.V.Godbole and V.K.Manchanda, National Symposium on Glass and Ceramics-08, 15-17 Oct, 2008, Bhabha Atomic Research Centre, Mumbai
2. EPR Investigations of Cu incorporated barium borosilicate glass, R.M.Kadam, M. Mohapatra, A.K.Munshi, S.N.Tripathy, R.K.Mishra, C.P.Kaushik, S.V.Godbole and V.K.Manchanda, National Symposium on Glass and Ceramics-08, 15-17 Oct, 2008, Bhabha Atomic Research Centre, Mumbai\
3. EPR and PL investigations of Fe and Mn bearing Trombay waste glass **M. Mohapatra**, R.M.Kadam, B.S.Tomar, R.K.Mishra, C.P.Kaushik, Kanwar Raj, S.V.Godbole and V.K.Manchanda, National Symposium on Glass and Ceramics-08, 15-17 Oct, 2008, Bhabha Atomic Research Centre, Mumbai
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5. Positron annihilation and photoluminescence investigations on electron irradiated barium borosilicate glass, M Mohapatra, D Dutta, R M Kadam, P K Pujari, V G Katrani, R.K.Mishra, C P Kaushik, B S Tomar, S V Godbole and V K Manchanda, DAE-BRNS Symposium on Nuclear and Radiochemistry-2009 (NUCAR-09), SVKM's Mithibai College, Mumbai
6. ESR Investigations of gamma and electron beam irradiated Trombay waste base glass, **M Mohapatra**, R.M.Kadam, R.K.Mishra, C.P.Kaushik, S.V.Godbole, Kanwar Raj and V.K.Manchanda, International Seminar on Science and Technology of Glass Materials-09, March 16-19, Acharya Nagarjuna University, Guntur, AP



7. Photoacoustic Spectroscopic Investigations of Alkali Borosilicate Glass doped with Cu ions, A. R. Dhobale, **M. Mohapatra**, Mithlesh Kumar, C. P. Kaushik and S.V. Godbole, International Seminar on Science and Technology of Glass Materials-09, March 16-19, Acharya Nagarjuna University, Guntur, AP
8. Characterization of borosilicate glass as host matrix for high level waste, **M Mohapatra** and V K Manchanda, International Seminar on Science and Technology of Glass Materials-09, March 16-19, Acharya Nagarjuna University, Guntur, AP
9. Photoluminescence investigations of RE (Eu and Gd) ion containing Trombay Waste Glass, **M. Mohapatra**, R.M.Kadam, B.S.Tomar, R.K.Mishra, C.P.Kaushik, Kanwar Raj, S.V.Godbole and V.K.Manchanda, National Conference on Luminescence and its Applications-09, Feb 17-19, 2009, Central Glass and Ceramics Research Institute, Kolkata, WB
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12. Radiation induced changes in nuclear waste glass: use of Eu^{3+} as a luminescence probe, **M. Mohapatra** and S.V.Godbole, DAE-BRNS Symposium on Nuclear and Radiochemistry (NUCAR-2011) Feb 22-26, 2011, Geetham University, Vishakhapattanam, AP, India.
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1. Characterization of Borosilicate Based Nuclear Waste Glasses, **M. Mohapatra**, S.V.Godbole, B.S.Tomar and V.K.Manchanda, Emerging Trends in Radiochemical Sciences (ETRS), Editors: M.Mohapatra, P.N.Pathak, P.K.Mohapatra and V.K.Manchanda, BARC Publication, 2011



Name : **Dipak Kumar Baisnab**
Enrolment No. : PHYS02200704008
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Title : Investigations on the Charge Order Melting in $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ and its Influence on Superconductivity and Transport Behaviour of $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$ Thin Films

Abstract

This thesis examines the influence of charge order melting brought about by current, magnetic field and substrate induced strain in a $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ (PCMO) layer, on the superconducting behaviour of a $\text{YBa}_2\text{Cu}_3\text{O}_{7-d}$ (YBCO) layer, lying in its proximity. Charge order melting in PCMO results in the formation of Ferromagnetic (FM) conducting clusters dispersed in a matrix of Charge Ordered (CO) insulating PCMO film and affects the transport as well as superconducting behaviour in the YBCO layer placed in close proximity. It is shown that when a PCMO thin film is deposited on MgO substrate with substantial lattice mismatch, the resulting strain induces a charge order melting when the thickness of the PCMO film is lower than a threshold. A current induced CO melting in PCMO is seen to affect the superconducting and magnetotransport behaviour of the PCMO/YBCO bilayer. The magnetoresistance measurements on the bilayer show that the superconducting transition temperature (T_c) of YBCO is suppressed to lower temperatures with a progressive increase in the applied current. In addition, with increase in current, a hump like feature appears in the temperature dependence of electrical resistivity prior to the onset of the superconducting transition. These observations could be rationalized in terms of a model based on current and/or magnetic field induced charge order melting. Analysis of the data enables vortex pinning characteristics to be deduced based on a suitable model. PCMO/YBCO/PCMO trilayer structures have also been experimentally investigated and the complicated variation of the $R(T)$ data are explained using a similar model that has been used to understand the bi-layers.

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1. Intricacies of Strain and Magnetic Field Induced Charge Order Melting in $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ Thin Films Dipak Kumar Baisnab T. Geetha Kumary, A. T. Satya, Awadhesh Mani, J. Janaki, R. Nithya, L.S. Vaidhyanathan, M.P. Janawadkar, and A. Bharathi, Journal of Magnetism and Magnetic Materials, 323, (2011) 2823
2. Evolution of Ferromagnetic clustering in $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ and its effect on the Critical Temperature of $\text{YBa}_2\text{Cu}_3\text{O}_7$ thin film Dipak Kumar Baisnab T. Geetha Kumary, A. T. Satya, Awadhesh Mani, R. Nithya, L. S. Vaidhyanathan, M. P. Janawadkar and A. Bharathi, Journal of Applied Physics, 111 (2012) 113910
3. Current Dependent Proximity Effects in $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3/\text{YBa}_2\text{Cu}_3\text{O}_7$ Bilayer Dipak Kumar Baisnab T. Geetha Kumary, A. T. Satya, Awadhesh Mani, L. S. Vaidhyanathan, M. P. Janawadkar and A. Bharathi,, Journal of Nanoscience Letters 3:13 (2013)
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5. Effect of current induced charge-order melting of $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ in partially masked superconducting $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3/\text{YBa}_2\text{Cu}_3\text{O}_7$ bilayer film Dipak Kumar Baisnab, M. P. Janawadkar, L. S. Vaidhyanathan and A. Bharathi Journal of Applied Physics, (Accepted)



Conference

6. Strain Enhanced charge-order melting in $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ thin films Dipak Kumar Baisnab T. Geetha Kumary, A. T. Satya, Awadhesh Mani, J. Janaki, R. Nithya, L. S. Vaidhyanathan, M. P. Janawadkar and A. Bharathi AIP Conf. Proc. 1347 (2011) 199
7. Effect of Current Induced Charge Order Melting of $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$ on $\text{YBa}_2\text{Cu}_3\text{O}_7$ Thin Film Dipak Kumar Baisnab T. Geetha Kumary, A. T. Satya, Awadhesh Mani, R. Nithya, L. S. Vaidhyanathan, M. P. Janawadkar and A. Bharathi, AIP Conf. Proc. 1447 (2012) 675
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10. Synthesis of $\beta\text{-Ga}_2\text{O}_3$ nano-particles embedded in Nb matrix by radiofrequency co-sputtering. L.S. Vaidhyanathan, M.P. Janawadkar, D. K. Baisnab et. al, International Symposium on Materials Chemistry-2008, Mumbai (2-6th December, 2008).
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12. Synthesis and low temperature studies of the $\text{Fe}_{1+\delta}\text{Te}$ system J.Janaki, T.GeethaKumary, Awadhesh Mani, Dipak Kumar Baisnab et. al, DAE SSPS-2009
13. Resistivity of thin films of $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ and Multilayers of YBCO/ Ga_2O_3 L.S.Vaidhyanathan, D. K. Baisnab et. al, PLD-2007, DAE-BRNS 4th National Symposium on PLD of thin films & Nanostructured materials.
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15. Development and utilization of SQUID sensors M.P. Janawadkar, R. Baskaran, L S Vaidhyanathan, R Nagendran, K Gireesan, D. K. Baisnab et. al, East Asia Symposium on Superconductor Electronics held at IIT Delhi(Dec 11-15, 2007).



Name : **Priyada P.**
Enrolment No. : PHYS02200804005
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Gamma Ray Scattering Non Destructive Evaluation Studies

Abstract

This paper focuses on the fluid-fluid, fluid-air interface level detection and density determination by gamma scattering method and intercomparison with transmission (gammatography) technique. The Monte Carlo (MC) numerical simulation of the scattering phenomena is done using the MCNP code. The obtained accuracies and resolution of the level detections and density measurements are higher in case of gamma scattering method compared to transmission method.

Publications

List of publications in referred international journals

1. P. Priyada, M. Margret, R. Ramar, Shivaramu, M. Menaka, L. Thilagam, B. Venkataraman, Baldev Raj, "Intercomparison of Gamma Scattering, Gammatography and Radiography Techniques for Mild Steel Nonuniform Corrosion Detection", Review of Scientific Instruments. 82(3), 035115 (2011)
2. P. Priyada, M. Margret, R. Ramar, Shivaramu, "Intercomparison of gamma ray scattering and transmission techniques for fluid-fluid and fluid-air interface levels detection and density measurements", Applied Radiation and Isotopes, 70 (3), 462-469 (2012)
3. P. Priyada, R. Ramar, Shivaramu, "An improved Compton scattering method for determination of concentration of solutions", Applied Radiation and Isotopes, 70 (10), 2421-2427 (2012)
4. P. Priyada, R. Ramar, Shivaramu, "Application of gamma ray back-scattering technique for non-destructive evaluation of voids in concrete", Applied Radiation and Isotopes, 74, 13-22 (2013)
5. P. Priyada, R. Ramar, Shivaramu, "Determining the water content in concrete by gamma scattering method", (Communicated to Annals of Nuclear Energy)
6. P. Priyada, R. Ramar, H. Krishnan, S. Viswanathan, Shivaramu, "Gamma photon techniques for detection of nucleation in super-heated emulsion detectors for neutron dosimetry", (Communicated to Radiation Protection Dosimetry)

List of conference papers

1. P. Priyada, M. Margret, R. Ramar, M. Menaka, Shivaramu, B. Venkataraman and Baldev Raj, Inter Comparison of Gamma Scattering with other NDE Techniques for MS Corrosion Detection, NDE-2010 Kolkata.
2. Shivaramu, P. Priyada, M. Margret, R. Ramar, Intercomparison of gamma ray scattering and transmission techniques for fluids interface level and density determination, Accepted for Oral Presentation and available online, 5th Pan American Conference for NDT, Mexico.
3. P. Priyada, M. Margret, R. Ramar and Shivaramu. Intercomparison of gamma ray scattering and transmission techniques for fluids interface level and density determination, NDE-2011 Chennai.
4. P. Priyada, R. Ramar and Shivaramu, Intercomparison of gamma scattering and transmission techniques for measurement of water content in concrete, Nineteenth National Symposium on Radiation Physics (NSRP19), 2012, Mamallapuram, Chennai.



Name : **Priya Maheshwari.**
Enrolment No. : CHEM01200904007
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Gamma Ray Scattering Non Destructive Evaluation Studies

Abstract

The thesis titled "Study of Nanoscale materials using positron Annihilation Spectroscopy" Mainly involves the study of nanoscale materials viz. nanopores in porous materials and nanoscale thin films using positron annihilation spectroscopy (PAS). The objective of the study has been two fold viz (i) investigation of materials at nanoscale using PAS and (ii) understanding the positron/Ps dynamics in these systems. The nanopores of zeolite and saponite clay have been employed as confining media for liquids (ethylene glycol, isopropanol and water) and the phase transition of the nanoconfined liquids has been investigated. The work highlights the role of interfacial interaction on the shift in the freezing/melting behavior of confined liquids. A new experimental evidence of the presence of transition at a temperature above the bulk freezing temperature of water, in addition to the known low temperature transition, has been shown. The work also includes depth profiling study using slow positron beam technique for the investigation of pore architecture in porous membranes as well as nanostructure characterization in ultra thin organic semiconductor (OSC) films. The porous membranes have been characterized for the pore interconnectivity which is an essential aspect in relation to transport properties of the membranes and is difficult to be obtained by conventional techniques. A correlation between Ps diffusion length and permeability of membranes has been established.

The work related to OSC thin films reveals the sensitivity of slow positron beam technique for nanostructure characterization of these films especially structural inhomogeneities and buried interfaces. The study on multilayer films has shown the presence of distinct interfaces between different organic and inorganic materials which otherwise, can not be probed by other techniques not destructively. This opens an avenue for slow positron beam characterization of OSC films in actual device configuration. It is also observed that positron mobility is comparable to chargecarrier mobility in these films. This has important implication in organic electronic industry where structural characterization using this technique at early stage of fabrication can give preliminary idea about the charge mobility which is an important parameter for highperformance devices. For this, the defect structure of OSC thin films as a function of different growth parameters is also studied. Interfacial characterization of engineered dielectric surfaces has also been carried out. Other complementary techniques such as NMR, dielectric relaxation spectroscopy and X-ray reflectivity have also been used to support the result.

Publications

1. Study of iron phthalocyanine organic semiconductor thin films using slow positron beam P. Maheshwari, D.Dutta, S. Samanta, A. Singh, D.K. Aswal, A. V. R. Reddy and P.K. Pujari *Phys. Stat. solidi c* 6,11, (2009)2589-2591.
2. Microstructure study of supported liquid membranes using slow positron beam P.K. Pujari, P. Maheshwari, S. K. Sharma, D. Dutta, K. Sudarshan and A. V. R. Reddy *Phys. Stat. solidi c* 6,11, (2009)2417-2419.



3. Effect of interfacial hydrogen bonding on the freezing/melting behavior of nano-confined liquids P. Maheshwari, D. Dutta, S. K. Sharma, K. Sudharshan, P. K. Pujari, M. Majumdar, B. Pahari , B. Bandyopadhyay, K. Ghosharay and A. Ghosharay *J. Phys. Chem C* 114 (2010) 4966.
4. Study of interfaces in organic semiconductor heterojunctions P. Maheshwari, D. Dutta, K. Sudarshan, S. K. Sharma, S. Samanta, A. Singh, D. K. Aswal and P. K. Pujari, *Journal of Physics: Conference Series* 262(2011) 012036.
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6. Phase Transition of water confined in Saponiates using Positron annihilation spectroscopy Priya Maheshwari, S. K. Sharma, D. Dutta, K. Sudarshan, P.K. Pujari *Mat. Sci. Forum*, 733(2013)111.
7. Phase transition of nanoconfined water in clay: Position annihilation, Nuclear magnetic resonance and Dielectric relaxation studies Priya Maheshwari , P. K. Pujari, S. K. Sharma, D. Dutta, K. Surdarshan, V. S. Mithu, P. K. Madhu, S. K. Deshpane, P. . Patil and N. Raje *J.Phys. Chem.* (Communicated)
8. Direct evidence of linkage between pore interconnectivity and permeability of metal ions in PTFE supported liquid membranes:A slow positron beam study Priya Maheshwari, D. Dutta, K. Sudarshan, S. K. Sharma, P. K. Mohapatra, P. U. Sastry and P. K. Pujari (Manuscript under Preparation)
9. Depth dependent inhomogeneities in nanosclae OSC films: PAS and XRR study Priya Maheshwari, D. Bhattacharya, S. K. Sharma, S. Mukherjee, S. Basu and P. K. Pujari (Manuscript under preparation)



Name : **Jayanta Mondal.**
Enrolment No. : PHYS01200704017
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Studies of Niobium and Development of Niobium Resonant RF Cavities for Accelerator Driven System

Abstract

The present approach for the fabrication of superconducting radio frequency (SRF) cavities is to roll and deep draw sheets of polycrystalline high-purity niobium. Jefferson Laboratory pioneered the use of large-grain/single-crystal Nb directly sliced from an ingot for the fabrication of single-crystal high-purity Nb SRF cavities. The large grain/single crystal niobium has several potential advantages over the polycrystalline niobium has become a viable alternative to the standard fine grain (ASTM grain size $>6 \mu\text{m}$), high purity ($\text{RRR} \geq 250$) niobium for the fabrication of high-performance SRF cavities for particle accelerators.

Niobium metal superconductivity in SRF accelerators is a nanoscale, near surface phenomena because of small RF penetration depth of the order of 10 – 100 nm. The cavity performance improvement over the 3-4 decades strongly indicates the topography and the chemistry of the inner surface impacts the final cavity performance.

Present day cavity preparation chemistry for the inner surface follow two different routes namely buffered chemical polishing (BCP) and electropolishing (EP). In the present thesis the studies are carried out with BCP surface treatment and EP route is not explored.

It has been known for quite some time that the low temperature baking (LTB) ($100 - 140^\circ\text{C}$) is a necessary final preparation stage to achieve high accelerating gradients in niobium RF cavity. Till date there exist different models to understand the LTB effect on niobium RF cavity, although any of them is not complete in a sense which can explain all the experimental observations.

An attempt has been made to study the material and superconducting properties of large grain niobium of different RRR value. In the present study the large grain samples are treated with BCP followed by different post purifications such as 600°C annealing, low temperature baking (LTB) in the range of $100 - 140^\circ\text{C}$. To understand the low temperature baking improvement of cavity performance experimental studies of surface magnetization are carried out. Also the study of positron annihilation spectroscopy shows a correlation of defect density dependence before and after annealing. The performance of SRF cavity is mostly described by the dependence of the unloaded quality factor Q_0 with accelerating electric field E_{acc} . Several past experiments had shown that there is a continuous degradation of Q_0 with E_{acc} (or peak magnetic field B_p) in the range of 20 – 100 mT. This phenomenon is termed as 'medium field Q-slope'. The present study includes the prototype single cell low beta cavity design, fabrication, EB welding and low temperature RF test at 2K. In this study also the medium field Q-Slope has been analyzed with the help of an added non linear term in Heabel's analytical model and a linear increase of surface resistance R_s with the magnetic field.

Publications

Journal Publications

1. Mondal, G.Ciovati, K.C.Mittal, G.R.Myneni. (2012). "Thermal conductivity of large grain niobium and effect of trapped vortices in the temperature range 1.8-5K" *Pramana-Journal of Physics*, 635, 78(4), (2012)



2. J. Mondal, G. Ciovati, P. Kneisel, K. C. Mittal and G. R. Myneni (2011). "Design, fabrication, RF test at 2K of 1050 MHz, $\beta = 0.49$ single cell large and fine grain niobium cavity", Journal of Instrumentation, 6 – T11003, JINST, 2011.doi:10.1088/1748-0221/6/11/T11003.
3. Amitava Roy, J. Mondal and K.C. Mittal (2008). "RF properties of 1050 MHz, $\beta = 0.49$ Elliptical cavity for High Current Proton Acceleration", Journal of Instrumentation, 3-P04002, JINST, 2008.

Conference Publications

1. J. Mondal, K.C.Mittal, G.Ciovati, P.kneisel, G.R.Myneni, "Characterization of Ingot Materials for SRF Cavity Production", Proceedings of SRF2009, Berlin, Germany, THOAAU01, Page: 455-461.
2. J. Mondal, T.K.Saha, S.Sarkar, S.B.Jawale, R. S. Vohra, A.V.Bapat, "Design, fabrication, room temperature RF test of 1050 MHz, $\beta = 0.49$ single cell large grain niobium cavity", International Vacuum Symposium-2012, VECC, Kolkata.
3. T.K.Saha, J. Mondal, K.C.Mittal, K.G.Bhushan and A.V.Bapat, "Fabrication of niobium superconducting accelerator cavity by electron beam welded joints" International Vacuum Symposium-2012, VECC, Kolkata.



Name : **Bibhuti Bhusan Mishra**
Enrolment No. : LIFE01200604010
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Studies on Polyphenol Oxidase in Brinjal (*Eggplant*; *Solanum melongena*)

Abstract

Polyphenol oxidase (PPO) catalyzes oxidation of phenolics resulting in post-processing browning in many cut fruits and vegetables including brinjal, which is a major hurdle in the success of minimally processed products in food industry. The thesis is organized into six chapters which include detailed studies on PPO activity, phenolic content, browning index, and polymorphism in PPO gene in eight cultivars of brinjal. The brinjal cultivars showed significant difference in PPO activity, phenolics content and browning. In fresh brinjal samples both PPO as well as phenolics were found to be equally important for browning. Browning was always found to be maximally correlated with phenolics but not with PPO in case of stored samples, indicating the major role of phenolics in post-cut browning. The chlorogenic acid was found to be the major phenolic with range of ~50-70% of total phenolics. A physical method which causes minimum mechanical injury (shown using Fluorescence and SEM studies) was developed to inhibit browning in fresh cut brinjal during storage. Shelf life of fine blade-cut, water dipped, and packaged brinjal increased up to 16 days at 4 °C. Two isoforms of PPO was observed in eight cultivars of brinjal. One isoform of PPO (PPO2) was 259 fold purified from 'Kalpatharu' cultivar using standard chromatographic procedures and its kinetic parameters were characterized. The purified PPO2 showed highest specificity towards 4-methyl catechol with very low Km (0.34 mM) and high catalytic efficiency (3.3×10^6). The active PPO was found to be homodimer of 112 kDa molecular weight. Among many natural and synthetic inhibitor studied, cysteine hydrochloride has shown good promise as a superior inhibitor with very low inhibitor constant of 1.8 μ M. The PPO genes in six cultivars were sequenced and were found to show significant level of homology. Two cultivars displaying highest PPO activity differed in the 38 amino acid stretch before copper B binding region. PPO gene of one of the cultivars was also cloned and expressed in *E.coli* BL21(DE3). The recombinant protein was purified and mol. wt. was found to be of 66 kDa, which comprises of signaling sequence of about 10 kDa. Present work describes the novel findings characterizing PPO from brinjal and its possible inhibition which could be an important mean to control post processing browning in minimally processed fruits and vegetables including brinjal.

Publications

1. Mishra, B. B., Gautam, S., Sharma, A. (2012). Browning of fresh-cut eggplant: Impact of cutting and storage. *Postharvest Biol. Technol.* 67, 44-51.
2. Mishra, B. B., Gautam, S., Sharma, A. (2012). Purification and characterization of native polyphenol oxidase (PPO) from eggplant (*Solanum melongena*). *Food chem.* 134, 1855–1861.
3. Mishra, B. B., Gautam, S., Sharma, A. (2013). Free phenolics and activePPO: The two major factors affecting post-cut browning in eggplant. *Food Chem*, 139(1-4), 105-114.

Posters presentations and awards

1. Mishra, B. B., Gautam, S., Sharma, A. (2012). Characterization of Polyphenol oxidase (PPO) from Brinjal. DAE-BRNS LSS-2012, Mumbai. December 17-19, 2012. (Best Poster award).
2. Mishra, B. B., Gautam, S., Sharma, A. (2012). Inhibition of browning and PPO activity in ready-to-cook eggplant. ICFOST XXI. Pune. January 20-21, 2012.



Name : **Saikat Kumar Nandy**
Enrolment No. : CHEM01200804018
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Novel Synthesis and Purification Process for PET-Radiopharmaceuticals for Rapid and Convenient Production

Abstract

The Ph.D thesis, "Novel Synthesis and Purification Technique for PET-Radiopharmaceuticals for Rapid & Convenient Production" submitted by Shri Saikat Kumar Nandy (CHEM 01 2008 040018) is based on developing novel strategies for simplifying the production of ^{18}F -labeled non-FDG PET Radiopharmaceuticals for oncology-imaging where [^{18}F]-FDG is not useful or lacks specificity. The thesis begins with the adaptation and optimization of a commercial, fully automated synthesis module meant for the production of ^{11}C -Methoinine to a General Purpose Fluorination Module, which was subsequently utilized for the production of ^{18}F -PET Radiopharmaceuticals, other than ^{18}F -FDG, by successfully developing solid phase extraction (SPE) purification techniques after understanding the synthesis-chemistry and the possible impurities. Three non-FDG PET radiopharmaceuticals namely [^{18}F]NaF (for skeletal imaging and bone metastasis), [^{18}F]FLT (for imaging cellular proliferation and brain tumour) and [^{18}F]FMISO (for tumour hypoxia imaging) have been produced and cleared by the DAE-Radiopharmaceutical Committee (RPC), for routine production and supply as radiopharmaceuticals. Their processes have been published in peer reviewed journals and cited by others. These have been used by nuclear medicine centres for the diagnosis and management of cancer patients over the last three years. Other promising ^{18}F -labelled PET radiotracers have been produced using novel SPE cartridge based purification and two of them viz., [^{18}F]FAZA (for tumour hypoxia imaging) and [^{18}F]FES (for Estrogen receptor +ve breast cancer imaging) are submitted to RPC for clearance. Others under various stages of development are [^{18}F]Fluoroacetate (for imaging prostate cancer), [^{18}F]Fluoroethyl acetate (for glial cell metabolism), [^{18}F]FHBG (for HSV tk-1 based viral infection imaging and gene therapy).

Publications

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2. Evaluation of the radiochemical impurities arising during the competitive fluorination of nosyl group during the synthesis of 3'-deoxy-3'-fluorothymidine, [^{18}F]FLT. S.K.Nandy, N.V. Krishnamurthy, M.G.R. Rajan. Journal of Radioanalytical & Nuclear Chemistry., 2010, 283, 245-251.
3. Fully automated and simplified radio synthesis of [^{18}F] 3'-Deoxy-3'-Fluorothymidine using Anhydro Precursor and Single Neutral Alumina Column Purification. S.K.Nandy, M.G.R.Rajan. Journal of Radioanalytical & Nuclear Chemistry., 2010, 283, 741-748.
4. The possibility of a fully automated procedure for radiosynthesis of fluorine-18-labeled fluoromisonidazole using simplified single, neutral alumina column purification procedure. Saikat Nandy, M.G.R.Rajan, A. Korde, N.V. Krishnamurthy. Applied Radiation and Isotopes., 2010, 68, 1937-1943.
5. Fully automated radiosynthesis of [^{18}F]Fluoromisonidazole with single neutral alumina column purification: optimization of reaction parameters. S.K.Nandy, M.G.R.Rajan. Journal of Radioanalytical & Nuclear Chemistry., 2010, 286, 241-248.
6. Simple, column purification technique for the fully automated radiosynthesis of [^{18}F]Fluoroazomycin-araboside ([^{18}F]FAZA). S.K.Nandy, M.G.R.Rajan. Applied Radiation and Isotopes., 2010, 68, 1944-1949.
7. Chondroid hamartoma presenting as solitary pulmonary module: Results of dual time point ^{18}F -fluorodeoxyglucose-PET and comparison with ^{18}F -fluorothymidine PET and histopathology.



Basu S., Nandy S., Rajan M.G.R., Ramadar M., Moghe S.
Hellenic Journal of Nuclear Medicine., 2011, 14.(correspondence)

International Journals (Abstracts)

1. Rapid synthesis of [^{18}F] Fluoro-L-Thymidine with simplified purification using a combination-column. S.K.Nandy, M.G.R.Rajan, A. Korde, P.R.Chaudhari & P.S.Soni. Journal of Labelled Compounds and Radiopharmaceuticals., 2007, 50 (S1), pp S1-S510, P 033.
2. Low cost combination-column for the purification of ^{18}F -FDG produced either by acid or alkali hydrolysis. S.K.Nandy, M.G.R.Rajan & P.S.Soni. Quarterly Journal of Nuclear Medicine and Molecular Imaging., 2008, 52 (S1).
3. Production of [^{18}F]Fluoromisonidazole with a single purification step using neutral alumina column: QC and Bio-distribution study: S.K.Nandy, M.G.R.Rajan & P.S.Soni. Quarterly Journal of Nuclear Medicine and Molecular Imaging., 2008, 52 (S1).
4. Radiochemical Analysis of [^{18}F]Fluorothymidine produced from BOC-precursor and purified with a combination column of anion-exchanger and alumina. S.K.Nandy, N.V. Krishnamurthy and R.M.Rajan. Journal of Labelled Compounds and Radiopharmaceuticals., 2009, 52 (S1), S256-S320, P 202.
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1. Synthesis of [^{18}F]Fluoromisonidazole using a general-purpose fluorination Module and combination purification column. S.K.Nandy, M.G.R.Rajan, A.Korde & P.S.Soni IAEA-CN-157/025, International conference on Clinical PET and Molecular Nuclear Medicine (IPET 2007), Bangkok, 10-14 November (2007).
2. Preliminary studies on a rapid radiosynthesis procedure for [^{18}F] FHBG using a Non-HPLC technique. S.K.Nandy, M.G.R.Rajan, A.Korde & P.S.Soni. IAEA-CN-157/025, International conference on Clinical PET and Molecular Nuclear Medicine (IPET 2007), Bangkok, 10-14 November (2007).
3. Multipurpose synthesis modules for preparing [F-18]-labeled compounds. M.G.R.Rajan, S.K.Nandy & P.S.Soni. IAEA-CN-157/025, International conference on Clinical PET and Molecular Nuclear Medicine (IPET 2007), Bangkok, 10-14 November (2007).
4. A simple and one pot fully automated synthesis of 3'-deoxy-3'-[^{18}F]fluorothymidine. S.K.Nandy, M.G.R.Rajan. IAEA-CN-185/148, International conference on Clinical PET and Molecular Nuclear Medicine (IPET 2011), Vienna, 8-11 November (2011).
5. A fully automated radiosynthesis of 4-[F-18]fluorobenzaldehyde: a synthon for amine-oxy peptide labelling. S.K.Nandy, M.G.R.Rajan. IAEA-CN-185/147, International conference on Clinical PET and Molecular Nuclear Medicine (IPET 2011), Vienna, 8-11 November (2011).
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7. A single column purification technique for the fully automated radiosynthesis of [F-18]Ethyl Fluoroacetate([F-18]EFA) as a proradiotracer of [F-18]fluoroacetate([F-18]FA) for the measurement of glial metabolism by PET. S.K.Nandy, M.G.R.Rajan. IAEA-CN-185/163, International conference on Clinical PET and Molecular Nuclear Medicine (IPET 2011), Vienna, 8-11 November (2011).



Name : **Nihar Ranjan Sahoo**
Enrolment No. : PHYS04200904002
Constituent Institute : Variable Energy Cyclotron Centre, Kolkata
Title : Probing the QCD Critical Point by Higher Moments of the Net-Charge Distribution at RHIC Energies

Abstract

The critical point occupies a significant position in the QCD phase diagram. The current Lattice QCD calculations reveal that, at the QCD Critical End Point (QCEP), fluctuations in conserved quantities like net-baryon, net-strangeness diverge. Higher, non-Gaussian, moment (like skewness, kurtosis, etc.) of these fluctuations are significantly more sensitive to the proximity of the QCEP. The non-Gaussianity (non-zero skewness and kurtosis) of the above observables increase if the system approaches towards QCEP. And also these higher moments are related to the correlation length, which diverges at QCEP. This divergence of correlation length infers Long Range Correlation in the system. Hence if our Lattice QCD calculations are in right track, then variation of Higher moments of net-charge distribution with energy ($\sqrt{s_{NN}}$) could give a strong evidence for the location of QCEP. This will be studied by the RHIC energy scan in the STAR experiment.

Our group has installed the photon multiplicity detector (PMD) in the STAR experiment. Photon production will be studied for different energies using the PMD. Photon multiplicity fluctuations may reveal important information about the critical point.

Publications

1. Beam energy dependence of higher moments of the net-charge multiplicity distributions in Au+Au collisions at RHIC Target Journal: Physical Review Letters (Collaboration Review)
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7. Probing the QCD critical point by higher moments of the net-charge and net- proton multiplicity distribution in STAR Experiment Nihar R. Sahoo (for the STAR Collaboration), Proceedings of the DAE Symp. on Nucl. Phys. 57 (2012)
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11. Third Harmonic Flow of Charged Particles in Au+Au Collisions at $\sqrt{s_{NN}} = 200$ GeV STAR Collaboration (L. Adamczyk et al.), Phys. Rev. C 88 (2013) 014904;
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Title : Antimony Adsorption and its Inhibition of Carbon Steel and Magnetite Surfaces in Chemical Decontamination Process

Abstract

In many nuclear power plants, particularly Pressurized Water Reactor and Pressurized Heavy Water Reactors, radioactive antimony (^{122}Sb & ^{124}Sb) is observed to be adsorbed on the magnetite coated carbon steel (CS) surface during chemical decontamination. The chemical decontamination is a process to dissolve the oxides housing radioactive nuclides and sized them on a cation-exchange column. The chemical decontamination is followed here using an acidic solution under de-aerated condition at 85°C . In this thesis, an attempt were made to explore the Sb (III) adsorption mechanism on CS and Fe_3O_4 surfaces, as well as Sb (III) adsorption reduction on these surfaces under defined chemical decontamination conditions.

Antimony (III) is sorbed on the CS surface by forming Fe-O-Sb surface complex and surface precipitation as amorphous FeSb_2O_4 and Sb^0 due to redox reaction between Sb(II) and Fe^0 . The iron dissolution promotes Sb (III) adsorption on Cs surface. Hence, the iron dissolution inhibition can prevent Sb (III) adsorption on CS surfave. Pickling type organic caorrosion inhibitor Rodine 92B and passivator type corrosion inhibitors MoO_4^{2-} & SeO_3^{2-} showed reduction in Sb (III) adsorption. Rodine 92 B and MoO_4^{2-} corrosion inhibitors reduced adsorption via preferentially adsorption on CS surface compared to Sb(III) and adsorption mechanism is similar to Sb (III) adsorption on CS surface.

In acidic solution, protonized surface hydroxyl (SOH) funcatgional groups on Fe_3O_4 play a vital role in the adsorption of Sb (III) on Fe_3O_4 surface. These protonized SOH groups attract Sb(III) oxyanions Coulombically and make primary surface complex due to condensation or continuous release of Fe from Fe_3O_4 surface even after complete adsorption of Sb(III) and it is released in the form of ligand-Fe-O-Sb complex instead of free Sb(III). Tartaric Acid(TA) gave minimum Sb(III) adsorption on Fe_3O_4 due to its maximum complexation possibilty with Sb(III) in solution. Subsequent studies were carried out with TA and Fe_3O_4 to reduce further Sb(III) adsorption. Antimony (III) adsorption was increased with TA and Fe_3O_4 to reduce further oxyanions such as MoO_4^{2-} or cations such as Mn^{2+} . The changes in the adsorption were explained in therms of the iron dissolution, which in turn influences the abundance of the SOH group. The presence of another complexing agent particularly phenanthroline along with TA reduced the Sb(III) adsorption. An attempt was made to chemically modify the SOH by adding Lauric acid or benzoic acid in solution, the adsorption process only delayed without changing much the quantity of saturation adsorption of Sb on Fe_3O_4 surface.

Sb(III) adsorption on thick Fe_3O_4 coated CS surface resembles Sb(III) adsorption on Fe_3O_4 powder whereas with thin Fe_3O_4 coated CS the process is similar to Sb(III) adsorption on CS surface. In case of thin Fe_3O_4 coated CS surface, MoO_4^{2-} showed minimum Sb(III) adsorption.

In nuclear power plants, thicker Fe_3O_4 coating on the CS surface is seen at some regions whereas thin coating is also seen at some places. As our studies showed that MoO_4^{2-} could prevent Sb(III) adsorption on thin Fe_3O_4 coated CS and the plain CS surface while TA is effective on Fe_3O_4 surface, so a combination of MoO_4^{2-} and TA could prevent Sb(III) adsorption over the entire range of Fe_3O_4 and CS surfaces.



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Title : Superconductivity in $\text{BaFe}_{2-x}\text{Ru}_x\text{As}_2$ System and Investigation of its Critical Properties

Abstract

The thesis work reports results on the first observation of superconductivity in $\text{BaFe}_{2-x}\text{Ru}_x\text{As}_2$ system and investigation of its critical properties. Based on the measured variation in spin density wave transition temperature (T_{SDW}) and superconducting transition temperature (T_{C}) versus Ru-concentration (x), a $T_{\text{SDW}}/T_{\text{C}}$ vs. x phase diagram has been proposed. Band structure calculations have been performed that indicate a reduction in Fe moment with Ru substitution that is in agreement with low temperature Mossbauer experiments. Results of the detailed study of the structural parameters, orthorhombic distortion and their correlation with superconductivity in the $\text{BaFe}_{2-x}\text{Ru}_x\text{As}_2$ system are presented.

The critical properties viz., upper critical fields and critical current density have been measured on single crystals in fields up to 16 T applied parallel and perpendicular to the c -axis of crystals. Anisotropy in upper critical field ($H_{\text{C}2}$), critical current density $J_{\text{c}}(H)$, and pinning properties have been measured and vortex phase diagram has been established. The critical current density and pinning properties have been measured for several samples with different Ru content across the superconducting dome in the Ru- substituted samples. The nature of superconducting fluctuations present prior to the onset of superconductivity has been analyzed based on scaling of excess magnetization and para-conductivity close to the mean-field superconducting transition temperatures, these points to three dimensional superconductivity in the system.

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Title : Study of Shear Driven Electron Magnetohydrodynamic (EMHD) Instabilities in Plasmas

Abstract

Present thesis is a study on the instabilities driven due to the shear in equilibrium electron current using Electron Magnetohydrodynamic (EMHD) model of plasma. These are the instabilities of sheared electron current configurations formed in a variety of physical situations e.g., fast z-pinch, fast ignition phenomena of laser fusion, collision less magnetic reconnections, plasma opening devices, inter planetary current-carrying plasmas etc. One of the key instabilities of these current configurations is the Kelvin Helmholtz (KH) instability, which has been mainly focused in the thesis.

KH instability is one of the prominent neutral fluid instability which destabilizes the interface of two fluids in relative motion under certain conditions. The EMHD system, in contrast to the neutral fluid system, contains natural length (electron skin depth) and time (whistler periods) scales associated to the electromagnetic character of electron fluid. As a major study, role these natural scales of EMHD have been investigated on KH instability in two dimensions. The perturbations are confined to the 2D plane consisting of shear and flow directions, in which the major action of KH instability lies. The self-consistent magnetic field, arising due to 2D sheared flow of electrons, is directed along the symmetry direction. It has been observed that the growth rate of the instability decreases as the shear width is increased in comparison to the electron skin depth. The instability is prominent only when the shear in the electron flow velocity is sharper than the electron skin depth. In order to understand the role of whistlers on the instability, a uniform external magnetic field B_0 has been introduced along the flow direction (in the plane of KH). The action of KH distorts the magnetic field to a sheared configuration. The tension caused due to the distortion tries to restore the magnetic field configuration and sets up oscillations at whistler frequency. The process of excitation of whistlers costs the energy and makes the KH instability less favourable. The linear analysis shows that the growth rate reduces as the magnetic field strength is increased. Nonlinear simulations have been carried out to understand the role of whistlers in the nonlinear regime of instability. The nonlinear state, in the absence of B_0 , is a coherent vortex occupying the box size. This is because of two non-dissipative square invariants namely, energy and enstrophy, supported by two dimensional EMHD model. However, in the presence of B_0 , the nonlinear state is significantly changed from the ordered state of $B_0 = 0$ case. The long scale structures are formed only along the direction of B_0 and there is hardly any extension in structures along the transverse direction. This induces anisotropy in the system. The observed anisotropy is a characteristic of the nonlinear cascade mediated by whistlers. Due to the anisotropic cascade, the KH instability induced mixing of the fluids, flowing in two directions, around the shear layer is less. Consequently, the flattening of shear layer is observed to be weaker.

In three dimensional regime of instability, local kink mode also exists in addition to KH mode. The kink mode requires finite electron inertia and is driven by the gradient in the equilibrium velocity, unlike the KH mode which is driven by the curvature in equilibrium velocity. The interplay of KH and kink modes has been studied for simple sheared flow as well as in the presence of external magnetic field. The linear studies indicate that the dominance of one mode over the other is determined by the three factors, (i) value of shear width in comparison with the electron skin depth, (ii) external magnetic field along the



flow direction and (iii) external magnetic field normal to the plane of flow and shear. Nonlinear simulations carried out are in the agreement with results from linear studies. The nonlinear state of 3D instability is found to be strongly turbulent, unlike the 2D case. Spectral cascade features have been analysed for the turbulence generated in the nonlinear state.

The shear driven instability processes have been investigated for the Isichenko solutions of EMHD equations, which are in the form of stationary monopoles and propagating dipoles. The structures are stable against the excitation of nonlocal KH mode as the unstable wavelengths are longer than the structure size. For kink mode, however, wavelengths smaller than the structure size are also unstable. It has been found that the structures indeed show destabilization due to kink mode in nonlinear simulation with monopoles and dipoles as the initial conditions.

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Name : **Monali Nitin Kawade**
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Title : Photodissociation Dynamics of Polyatomic Molecules in Gas-Phase

Abstract

1. Dynamics of N-OH Bond Dissociation in Cyclopentanone and Cyclohexanone Oxime at 193 nm: Laser-Induced Fluorescence Detection of Nascent OH (v'' , J'')

Monali N. Kawade, Ankur Saha, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik

Cyclohexanone oxime (CHO) and cyclopentanone oxime (CPO) in the vapor phase undergo N-OH bond scission upon excitation at 193 nm to produce OH, which was detected state selectively employing laser induced fluorescence. The measured energy distribution between fragments for both oximes suggests that in CHO the OH produced is mostly vibrationally cold, with moderate rotational excitation, whereas in CPO the OH fragment is also formed in $v''=1$ (~2%). The rotational population of OH ($v''=0$, J'') from CHO is characterized by a rotational temperature of 1440 ± 80 K, whereas the rotational populations of OH ($v''=0$, J'') and OH ($v''=1$, J'') from CPO are characterized by temperatures of 1360 ± 90 K and 930 ± 170 K, respectively. A high fraction of the available energy is partitioned to the relative translation of the fragments with f_T values of 0.25 and 0.22 for CHO and CPO, respectively. In the case of CHO, the Λ -doublet states of the nascent OH radical are populated almost equally in lower rotational quantum levels N'' , with a preference for Π^+ (A'') states for higher N'' . However, there is no preference for either of the two spin orbit states $\Pi_{3/2}$ and $\Pi_{1/2}$ of OH. The nascent OH product in CPO is equally distributed in both Λ -doublet states of Π^+ (A'') and Π^- (A'') for all N'' , but has a preference for the $\Pi_{3/2}$ spin orbit state. Experimental work in combination with theoretical calculations suggests that both CHO and CPO molecules at 193 nm are excited to the S_2 state, which undergoes nonradiative relaxation to the T_2 state. Subsequently, molecules undergo the N-OH bond dissociation from the T_2 state with an exit barrier to produce OH (v'' , J'').

2. Dynamics of Cl (2P_i) Atom Formation in the Photodissociation of Fumaryl Chloride (CICO—CH=CH—COCl) at 235 nm: A Resonance Enhanced Multiphoton Ionization (REMPI) Time-of-Flight (TOF) Study

Monali N. Kawade, Ankur Saha, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik, P. N. Bajaj

The photodissociation dynamics of fumaryl chloride (CICO—CH=CH—COCl) has been studied in a supersonic molecular beam around 235 nm using resonance enhanced multiphoton ionization (REMPI) time-of-flight (TOF) technique by detecting the nascent state of the primary chlorine atom. A single laser has been used for excitation of fumaryl chloride and the REMPI detection of chlorine atoms in their spin-orbit states, Cl ($^2P_{3/2}$) and Cl* ($^2P_{1/2}$). We have determined the translational energy distribution, the recoil anisotropy parameter, β , and the spin-orbit branching ratio for chlorine atom elimination channels. To obtain these, measured polarization-dependent and state-specific TOF profiles are converted into kinetic energy distributions, using a least-squares fitting method, taking into account the fragment recoil anisotropies, β_i . The TOF profiles for both Cl and Cl* are found to be independent of laser polarization; i.e., β is well characterized by a value of 0.0, within the experimental uncertainties. Two components, namely, the fast and the slow, are observed in the translational energy distribution, $P(E_T)$, of Cl and Cl* atoms, and assigned to be formed from different potential energy surfaces. The average translational energies for the fast components of the Cl and Cl* channels are 14.9 ± 1.6 and $16.8(1.6)$ kcal/mol, respectively. Similarly, for the slow components, the average translational energies of the Cl and Cl* channels are 3.4 ± 0.8 and 3.1 ± 0.8 kcal/mol, respectively. The energy partitioning into the translational modes is



interpreted with the help of various models, such as impulsive and statistical models. Apart from the chlorine atom elimination channel, molecular hydrogen chloride (HCl) elimination is also observed in the photodissociation process. The HCl product has been detected, using a REMPI scheme in the region of 236-237 nm. The observation of the molecular HCl in the dissociation process highlights the importance of the relaxation process, in which the initially excited parent molecule relaxes to the ground state from where the molecular (HCl) elimination takes place.

3. Laser-induced UV photodissociation of 2-bromo-2-nitropropane: Dynamics of OH and Br formation

Ankur Saha, Monali Kawade, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik

Photoexcitation of 2-bromo-2-nitropropane (BNP) at 248 and 193 nm generates OH, Br, and NO₂ among other products. The OH fragment is detected by laser-induced fluorescence spectroscopy, and its translational and internal state distributions (vibration, rotation, spin-orbit, and Λ -doubling components) are probed. At both 248 and 193 nm, the OH fragment is produced translationally hot with the energy of 10.8 and 17.2 kcal/mol, respectively. It is produced vibrationally cold ($v''=0$) at 248 nm, and excited ($v''=1$) at 193 nm with a vibrational temperature of 1870 ± 150 K. It is also generated with rotational excitation, rotational populations of OH($v''=0$) being characterized by a temperature of 550 ± 50 and 925 ± 100 K at 248 and 193 nm excitation of BNP, respectively. The spin-orbit components of OH ($X^2\Pi$) are not in equilibrium on excitation at 193 nm, but the Λ -doublets are almost in equilibrium, implying no preference for its π lobe with respect to the plane of rotation. The NO₂ product is produced electronically excited, as detected by measuring UV-visible fluorescence, at 193 nm and mostly in the ground electronic state at 248 nm. The Br product is detected employing resonance-enhanced multiphoton ionization with time-of-flight mass spectrometer for better understanding of the dynamics of dissociation. The forward convolution analysis of the experimental data has provided translational energy distributions and anisotropy parameters for both Br($^2P_{3/2}$) and Br*($^2P_{1/2}$). The average translational energies for the Br and Br* channels are 5.0 ± 1.0 and 6.0 ± 1.5 kcal/mol. No recoil anisotropies were observed for these products. Most plausible mechanisms of OH and Br formation are discussed based on both the experimental and the theoretical results. Results suggest that the electronically excited BNP molecules at 248 and 234 nm relax to the ground state, and subsequently dissociate to produce OH and Br through different channels. The mechanism of OH formation from BNP on excitation at 193 nm is also discussed.

4. Resonance Enhanced Multiphoton Ionization-Time of Flight (REMPI-TOF) study of phosphorous oxychloride (POCl₃) dissociation at 235 nm: dynamics of Cl (2P_j) formation

Ankur Saha, Monali N. Kawade, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik, P. N. Bajaj

In one-color REMPI-TOF experiment, the photodissociation dynamics of POCl₃ has been studied by photolyzing POCl₃ and probing the chlorine atom photofragments, namely, Cl($^2P_{3/2}$) and Cl*($^2P_{1/2}$) using 2+1 REMPI scheme, in the 234-236 nm region. We have determined the centre-of-mass photofragment speed distribution, recoil anisotropy parameter, and the spin-orbit branching ratio for chlorine atom elimination channels. The anisotropy parameters for Cl and Cl* are the same, and characterized by a value of 0.0 ± 0.05 . Two components, namely, the fast and the slow, are observed in the translational energy distributions of Cl and Cl*. The average translational energies for the Cl and Cl* channels for the fast components are 12.5 ± 1.5 and 16.8 ± 1.5 kcal/mol, while, for the slow components, the average translational energies are 1.5 ± 1.0 and 2.5 ± 1.0 kcal/mol, respectively. Apart from the chlorine atom elimination channel, Cl₂ elimination is also observed in the photodissociation of POCl₃.



5. Photodissociation Dynamics of Halogenated Thiophenes at 235 nm: A Resonance Enhanced Multiphoton Ionization-Time of Flight (REMPI-TOF) study

Monali N. Kawade, Ankur Saha, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik, P. N. Bajaj

The photodissociation dynamics of halogen-substituted thiophenes, namely, 2-chlorothiophene and 2-bromo-5-chlorothiophene, has been studied in a supersonic molecular beam around 235 nm, using resonance enhanced multiphoton ionization (REMPI) time-of-flight (TOF) technique, by detecting the nascent state of the primary halogen atoms. A single laser has been used for excitation of halothiophenes, as well as for the REMPI detection of photoproducts, namely, chlorine and bromine atoms, in their spin-orbit states $X(^2P_{3/2})$ and $X(^2P_{1/2})$. We have determined the translational energy distribution, the recoil anisotropy parameter, β , and the spin-orbit branching ratio, for chlorine and bromine atom elimination channels. State-specific TOF profiles are converted into kinetic energy distributions, using a least-squares fitting method, taking into account the fragment anisotropies, β_i . The TOF profiles for Cl, Cl*, Br, and Br* are found to be independent of laser polarization; i.e., the β is well characterized by a value of ~ 0.0 , within the experimental uncertainties. For 2-chlorothiophene, we have observed two components for the Cl and only one component for the Cl* atom elimination channel in the translational energy distributions. The average translational energies for the fast and the slow components of the Cl channel are 3.0 ± 1.0 and 1.0 ± 0.5 kcal/mol, respectively. For Cl*, the average translational energy is 3.5 ± 1.0 kcal/mol. For 2-bromo-5-chlorothiophene, we have observed only one component for Cl, Cl*, Br, and Br* in the translational energy distributions. The average translational energies for the Cl and Cl* channels are 3.5 ± 1.0 and 5.0 ± 1.0 kcal/mol, respectively, whereas the average translational energies for the Br and Br* channels are 2.0 ± 1.0 and 3.5 ± 1.0 kcal/mol, respectively. The energy partitioning into the translational modes is interpreted with the help of various models, such as impulsive and statistical models. The ΔH_{298}^f value for 2-chlorothiophene has been estimated theoretically to be 23.5 kcal/mol.

6. Photodissociation Dynamics of enolic 1,2-cyclohexane dione at 266, 248, and 193 nm: Mechanism and nascent state product distribution of OH study

Monali N. Kawade, Ankur Saha, Hari P. Upadhyaya, Awadhesh Kumar, and Prakash D. Naik, P. N. Bajaj

The photodissociation dynamics of 1,2-cyclohexanedione (CHD), which exists in enolic form in gas phase, is studied using pulsed laser photolysis (LP)-laser induced fluorescence (LIF) "pump-and-probe" technique at room temperature. The nascent state distribution of the OH radical, formed after initial photoexcitation of the molecule to it is (π , π^*) and Rydberg states, is determined. The initial (π , π^*) and Rydberg states are prepared by excitation with the fourth harmonic output of Nd:YAG (266 nm)/KrF (248 nm) and ArF (193 nm) lasers, respectively. The ro-vibrational distribution of the nascent OH photofragment is measured in collision-free conditions using LIF. The OH fragments are formed in the vibrationally cold state at all the above wavelengths of excitation but differ in rotational state distributions. At 266 nm photolysis, the rotational population of OH shows a curvature in Boltzmann plot, which is fairly described by two types of Boltzmann-like distributions characterized by rotational temperatures of 3100 ± 100 and 900 ± 80 K. However, at 248 nm photolysis, the rotational distribution is described by a single rotational temperature of 950 ± 80 K. The spin-orbit and Λ -doublets ratios of OH fragments formed in the dissociation process are also measured. The average translational energy in the center-of-mass coordinate, partitioned into the photofragment pairs of the OH formation channels, is determined to be 12.5 ± 3.0 , 12.7 ± 3.0 , and 12.0 ± 3.0 kcal/mol at 266, 248, and 193 nm excitation, respectively. The energy partitioning into various degrees of freedom of products is interpreted with the help of different models, namely, statistical, impulsive, and hybrid models. To understand the nature of the dissociative potential energy surface involved in the OH formation channel, detailed *ab initio* calculations are performed



using configuration interaction-singles (CIS) method. It is proposed that at 266 nm photolysis, the OH fragment is formed from two different excited state structures, one with a strong H bonding, similar to that in the ground state, and another without effective H bonding, whereas, at 248 nm photodissociation, it seems that the OH formation occurs mainly from the excited state, which lacks effective H-bonding. At 193 nm excitation, the initially prepared population in the Rydberg state crosses over to a nearby σ^* repulsive state along the C-O bond, from where the dissociation takes place. The exit barrier for the OH dissociation channel is estimated to be 14 kcal/mol. The existence of dynamical constraint due to strong hydrogen bond in the ground state is effectively present in the dissociation process at 266 and somewhat deficient at 248 nm photolysis.

7. Photoexcitation of 2-bromo-2-chloro-1,1,1-trifluoroethane (Halothane) to repulsive surface $n\sigma^*(C-Br)$ at 234 nm: Dynamics of C-Br and C-Cl bond rupture

Ankur Saha, Monali N. Kawade, Hari P. Upadhyaya, Awadhesh Kumar, and Prakash D. Naik
The photodissociation dynamics of 2-bromo-2-chloro-1,1,1-trifluoroethane (halothane) have been studied near 234 nm, in a molecular beam environment, employing resonance-enhanced multiphoton ionization with time-of-flight mass spectrometer (REMPI-TOF-MS). Both bromine and chlorine atoms are detected in both the ground and spin-orbit excited states. The C-Br bond scission is observed predominantly due to direct $\sigma^*(C-Br) \leftarrow n(Br)$ transition, with translational energy distribution described with a soft impulsive model. The recoil anisotropy parameter (β) of 0.6 ± 0.2 for this channel vindicates the impulsive nature of dissociation. The diabatic crossing from the $n\sigma^*(C-Br)$ surface to $n\sigma^*(C-Cl)$ diabatic surface is responsible for chlorine formation via the C-Cl bond fission, which is supported by the excited state molecular orbital calculations. The velocity distribution of bromine atom has one component, however, that of chlorine atom is bimodal. Both fast and slow chlorine atom channels, with the β value of 0.3 ± 0.1 , are produced impulsively from the $n\sigma^*(C-Cl)$ repulsive surface.

Publications

1. Monali N. Kawade, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik Photodissociation dynamics study of nitrocyclopentane at 193 nm and 2-chloro-6-nitrotoluene at 193, 248 and 266 nm. (to be communicated)
2. Ankur Saha, Monali Kawade, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik Photodissociation dynamics of benzyl chloride at 235 nm: Resonance-enhanced multiphoton ionization (REMPI) detection of Cl and HCl. (Communicated)
3. Ankur Saha, Monali N. Kawade, Hari P. Upadhyaya, Awadhesh Kumar, and Prakash D. Naik Photoexcitation of 2-bromo-2-chloro-1,1,1-trifluoroethane (Halothane) to repulsive surface $n\sigma^*(C-Br)$ at 234 nm: Dynamics of C-Br and C-Cl bond rupture, *Chem. Phys.*, 2013, 416,1-10 (not included in the thesis).
4. Monali N. Kawade, Ankur Saha, Hari P. Upadhyaya, Awadhesh Kumar, and Prakash D. Naik, P. N. Bajaj
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Laser-induced UV photodissociation of 2-bromo-2-nitropropane: Dynamics of OH and Br formation, *J. Chem. Phys.*, 2011, 134, 044316(not included in the thesis).
8. Monali N. Kawade, Ankur Saha, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik, P. N. Bajaj
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9. Monali N. Kawade, Ankur Saha, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik
Dynamics of N-OH Bond Dissociation in Cyclopentanone and Cyclohexanone Oxime at 193 nm: Laser-Induced Fluorescence Detection of Nascent OH (ν'' , J''), *J. Phys. Chem. A* 2010, 114, 12369-12377

List of symposium publications:

1. Monali N. Kawade, Yogesh Indulkar, Ankur Saha, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik
Ultraviolet photodissociation dynamics of hexachloro acetone at 235 nm, TSRP-2012, 4-7 January 2012, Multipurpose Hall, BARC Training School Hostel and Guest House, Anushaktinagar Mumbai, India.
2. Monali N. Kawade, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik
Photodissociation dynamics of 2-chloro-6-nitrotoluene at 193 and 248 nm, NLS-19, 1-4 December 2010, RRCAT, Indore, India
3. Ankur Saha, Monali N. Kawade, Hari P. Upadhyaya, Awadhesh Kumar, Prakash D. Naik, P. N. Bajaj
Dissociation Dynamics of Fumaryl Chloride: A REMPI-TOF Study, APSRC-TSRP-2010, 14-17 September 2010, Lonavala, India.
4. Monali Kawade, Awadhesh Kumar, Hari P. Upadhyaya, P. D. Naik
Dynamics of N-OH bond dissociation in cyclopentanone and cyclohexanone oxime at 193 nm: Laser Induced Fluorescence detection of nascent OH (ν'' , J''), SDMC, 18-21 February 2010, The International Center, Dona Paula, Goa, India.
5. S. SenGupta, M. Kawade, Y. Indulkar, A. Kumar, S. Dhanya, P. D. Naik, P. N. Bajaj
Kinetic study of the gas-phase reaction of $\text{CF}_3\text{CH}_2\text{OCH}_2\text{CF}_3$ with OH radical, NSRP-2009, 12-14 March 2009, Kumaun University, Nainital, India.



Name : **Debabrata Banerjee**
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Title : Waves and Instabilities in Inhomogeneous Strongly Coupled Dusty Plasma

Abstract

The contents of this thesis provides a detailed analytical and numerical study of low frequency waves and instabilities in a strongly coupled dusty plasma considering the effect of viscoelastic and non-Newtonian properties in presence of inhomogeneous dust shear flow. Because of large negative charge on each particle, neighbouring dust particles have strong coulomb coupling between them which develop long range correlation in the system. At low temperature, dusty plasma can stay in a state where both viscosity and elasticity are equally effective. Due to strong coupling, system can support shear wave like transverse wave in elastic string. In the refereed article [1], we have theoretically predicted the existence of magneto-elastic wave in strongly coupled magnetized dusty plasma similar to the magneto sonic mode in magnetized plasma. In the article [2], we have shown theoretically, that velocity shear rate dependence of viscosity (non-Newtonian property) could trigger instability of shear wave in presence of inhomogeneous dust shear flow. It is also interesting to study the nonlinear effect of these non-Newtonian property on shear wave. In a recent article [5], we have reported that nonlinearity coming from non-Newtonian effect causes recurrence behaviour of shear wave which has similarity with the famous FPU recurrence in vibrating sting with quadratic and cubic nonlinearity. In the article [6], we have studied Kelvin-Helmholtz instability of unbounded dust shear flow of hyperbolic tangent type in strong coupling limit and reported that elastic property enhances the growth rate of instability. We have also found that shear thickening property of dusty plasma stabilize the Kelvin-Helmholtz instability in a bounded dust flow. However, shear thinning property enhances the instability. This has been reported in the very recent paper in Physics of Plasma [7].

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7. D. Banerjee, S. Garai, M. S. Janaki and N. Chakrabarti, Physics of Plasmas, 20, 073702 (2013).



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Title : Phenomenological Consequences of QCD Bremsstrahlung Processes in RHIC and LHC

Abstract

Strong modification of the internal architecture of a jet shower, in the form of energy degradation of most energetic partons as well as effects on the transverse momentum broadening and in-jet gluon multiplicity, in general are governed by both inelastic and elastic processes. QCD based analytical analysis of quenching of jets remain clogged so far to soft and eikonal limits of parton kinematics. In this thesis I have addressed some key issues, for which the standard jet quenching models are still lacking. We recalled the light and heavy quarks scattering process in Feynman Gauge, instead of usually employed light-cone gauge. We derived a compact expression for gluon emission off a heavy quark through the scattering with a light parton. This improved expression is valid for the full range of rapidity of the radiated gluon i.e. free from small angle/collinear gluon emission approximation for soft gluon emissions. Our analysis shows that even though there is a suppression of radiative soft gluon emission due to the mass of the heavy quark in the forward direction, it is almost tantamount in the backward regions. Consequently present findings indicate that a heavy quark emits a soft gluon almost similar to that of a light quark. We then obtained the radiative energy loss of a heavy quark akin to the Bethe-Heitler approximation. To compute the nuclear suppression factor for D-meson we consider both radiative and collision energy loss along with longitudinal expansion of the medium. The nuclear modification factor for D-meson with radiative energy loss obtained in the present formalism has an increasing trend at high transverse momentum and found to agree closely with the very recent data from ALICE collaboration at 2.76 ATeV. Our results are in accordance with trends of R_{AA} both from RHIC as well as LHC. Since there is not a single adjustable parameters for us, the simultaneously good description of R_{AA} both at RHIC and at LHC in our model is rather encouraging.

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6. C. A. Islam, R. Abir, M. G. Mustafa, S. K. Ghosh and R. Ray. Accepted in J. Phys. G (2013).



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Title : Generalized Hydrodynamic Description of Dusty Plasmas

Abstract

Contents A plasma impregnated with heavier macroscopic sized dust particles, is termed as a dusty plasma when the charged (due to electron/ion impingement on the dust surface) dust species behaves in a collective manner. The typical low thermal velocity and high charge density on the macroscopic dust species often renders such a dusty plasma medium in a strongly coupled state. Such dusty plasmas can be prepared artificially and/or get formed inherently in certain laboratory situations, for example in Tokamaks, rocket exhausts, plasma torches etc. In addition they are also ubiquitously present in astrophysical environments such as Planetary ring systems, Stars, Solar nebulae etc.

In recent years, the dusty plasma medium has attracted a lot of attention due to its variety of applications and the possibility of it being able to address several interesting fundamental physics issues in a simpler setting. One of the main attributes in the case of the dusty plasma medium is the ease with which it can be prepared/found in a strongly coupled regime. In this regime, the dusty plasmas can mimic the physical characteristics of a broad range of fluids (simple viscous as well as elastic nature are exhibited) and crystalline solids as well. The description of such a fluid behavior (visco - elastic features) has been in the past provided by the Generalized Hydrodynamic (GHD) formulation for the understanding of the linear response of the medium. Such a study has revealed existence of a modified dispersion characteristics of dust acoustic waves and the existence of the transverse shear waves. These predictions have been experimentally verified and have also been reproduced by the MD (Molecular Dynamics) simulations.

The GHD model has been employed in this thesis to carry out investigations of the dusty plasma medium in the nonlinear regime. In particular the 1-D response of the medium has been explored by studying the permissible coherent solutions and their evolution. In 2-D the characteristics of shear flow driven Kelvin – Helmholtz (KH) instability has been studied extensively for this particular medium. The observation of small scale structure formation in the context of KH evolution has led us to a detailed investigation on studying spectral evolution of the turbulent fluctuations for this medium.

Some highlights of our investigation are:

- The observation of readily accessible and stable singular cusp structures dithering at the wave breaking point in our 1-D simulations for weakly coupled dusty plasma system.
- The weakly nonlinear strong coupling 1-D dusty plasma system has been shown to follow a novel paradigm of Hunter Saxton (HS) equation in contrast to the usual KdV equation followed by the system in the weak coupling limit. The HS equation is known not to permit smooth soliton solutions. The equations instead permit both conservative and dissipative singular shock solutions. This is a characteristic feature of elasticity in the medium. The evolution of the GHD equations in strong coupling 1-D limit also demonstrate the formation of shocks.
- In 2-D, the properties of the shear flow driven Kelvin - Helmholtz (KH) instability has been studied in detail. The compressibility and dispersion effects in the weak coupling case show a reduction in the growth rate and the domain of the unstable mode wave numbers are also found to shrink. These features are borne out in the nonlinear simulations. In the nonlinear state, the coalescence of smaller vortices ultimately lead to the formation of long scale vortex structures.



- In the strong coupling limit the growth rate curve is bound between the two curves involving the inviscid and viscous cases (with infinitesimal relaxation time) of the weak coupling case. These features of the growth are borne out in the simulations. In contrast to the weakly coupled case the nonlinear regime of the strongly coupled medium shows a novel phenomena of recurrence in which there is a repetitive formation of long scale structures interrupted by the appearance of short scales again and again. This observation show that the process of spectral cascade in the strong coupling regime has to be fairly complex.
- The spectral cascade features were studied by employing an initial spectrum of random fluctuations around speci_c regions of the wave numbers. It is observed that unlike the turbulent spectra of normal fluids, in this case, there cannot be any characterization in terms of a single power law. Instead one observes a break in the spectra, with different regions exhibiting different forms. The evolved spectrum also does not show any universality and has dependence on the initial content of the spectral excitations. These features are understood in terms of the memory relaxation parameter intrinsic to the GHD equation.

It is important to carry out further studies on the GHD depiction of the medium and constitutes the future scope of the thesis. Experimental confirmation of our observations would be interesting and important. The recent observation by Teng et al., on the singular cusp solutions are in line with our simulation studies [1]. However, other phenomena related to turbulent spectral cascade properties can be experimentally investigated.

Publications

Publications in Peer Reviewd Journals:

1. Sheared flow driven instability in Visco-Elastic fluids, Sanat Kumar Tiwari, Vikram Singh Dharodi, Amita Das, Bhavesh G. Patel and Predhiman Kaw Submitted
2. Turbulence simulation in visco-elastic medium, Sanat Kumar Tiwari, Vikram Singh Dharodi, Amita Das, Bhavesh G. Patel and Predhiman Kaw To be submitted
3. Exact propagating nonlinear singular disturbances in strongly coupled dusty plasmas, Amita Das, Sanat Kumar Tiwari, Predhiman Kaw and Abhijit Sen Under communication, New Journal of Physics
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5. Kelvin-Helmholtz instability in a strongly coupled dusty plasma medium, Sanat Kumar Tiwari, Amita Das, Dilip Angom, Bhavesh G. Patel, Predhiman K. Kaw Physics of Plasmas 19, 073703 (2012)
6. Kelvin - Helmholtz instability in a weakly coupled dust fluid, Sanat Kumar Tiwari, Amita Das, Predhiman Kaw and Abhijit Sen Phys of Plasmas 19, 023703 (2012)
7. Longitudinal singular response of dusty plasma medium in weak and strong coupling limits, Sanat Kumar Tiwari, Amita Das, Predhiman Kaw and Abhijit Sen Physics of Plasmas 19, 013706(2012)
8. Nonlinear wave propagation in strongly coupled dusty plasmas, B. M. Veerasha, S. K. Tiwari, A. Sen, P. K. Kaw, and A. Das Physical Review E 81, 036407 (2010)

Conferences/Schools:

International Participation

1. Observation of cusp structures in 1-D dusty plasma simulations. (Talk) Sanat Kumar Tiwari, Amita Das, Abhijit Sen and Predhiman Kaw ICOPS, Chicago, Illinois, 26th - 30th June, 2011.



2. Kelvin Helmholtz Instability in dusty plasmas.(Poster) Sanat Kumar Tiwari, Amita Das, Abhijit Sen and Predhiman Kaw ICPDP,Garmisch-Partenkirchen, Germany 15th - 20th May, 2011.
3. Elastic Turbulence: In context of dusty plasmas. (Poster) Sanat Kumar Tiwari, Vikram Singh Dharodi, Amita Das, Bhavesh G. Patel and Predhiman Kaw ICCPPNDS, IPR, Gandhinagar, India November 2012.
4. Sheared Flow Instability in Dusty Plasmas: Fluid and Particle Approach. (Poster) Sanat Kumar Tiwari, Amita Das, Bhavesh G. Patel and Predhiman Kaw School on Hands-On Research in Complex Systems, ICTP, Italy, 1-12 July 2013.

National Participation

1. Nonlinear Studies of strongly correlated dusty plasma system.(Talk) Sanat Kumar Tiwari, Amita Das, Abhijit Sen and Predhiman Kaw 24th National Symposium On Plasma Science and Technology, 8-11 Dec, 2009, Hamirpur, India.
2. Observation of various nonlinear structures in 1-D dusty plasma simulations. (Poster) Sanat Kumar Tiwari, Amita Das, Abhijit Sen and Predhiman Kaw 1st Scholar's Colloquium, IPR, Gandhinagar, India April 2011.
3. 2-D Turbulence in Strongly Coupled Dusty Plasmas. (Poster) Sanat Kumar Tiwari, , Vikram Singh Dharodi, Amita Das, Bhavesh G. Patel and Predhiman Kaw National Symposium on Plasma Science and Technology- Plasma-2012, Pondicherry University, India, December 2012.
4. Solitary structures Near wave breaking point in dusty plasmas. (Talk and Poster) Sanat Kumar Tiwari, Amita Das, Abhijit Sen and Predhiman Kaw 1st PSSI-Plasma Scholars Colloquium, IPR, Gandhinagar, India July 2012.



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Title : Regular Quantifiers in Logics

Abstract

First order logic on words is a well-studied logic. It is known that first order logic (FO) with a linear order, FO[<] (in our notation, we enclose the relations used in square bracket) cannot count more than a constant. From the result of Furst, Saxe and Sipser we know that, the logic FO[<, Arb] cannot define

$$L_{even} = \{w \in \{0, 1\}^* \mid \text{number of } 1 \text{ s is even in } w\}$$

Here Arb stands for arbitrary numerical predicates (predicates whose truth depends only on the position of the variables in the linear order and not on the letters at these positions). This shows that first order logic cannot count modulo a number (two in the language L_{even}). This inability to count, led to extending first order logic by different kinds of quantifiers.

In the thesis, we study logics on words extended with *regular* quantifiers. Modulo counting quantifiers, which have been well studied in the past, are examples of regular quantifiers. These quantifiers can be generalized to group quantifiers and further to monoid quantifiers, all being regular quantifiers.

The logics we extend can be classified into two parts. In the first part, we look at logics which define regular languages like FO[<] and linear temporal logic (LTL). We extend these logics with the above mentioned regular quantifiers. In the second part, we look at regular quantifiers over a linear order and an addition function which respects the linear order. This takes us outside regular languages. We ask the following questions about the logics we consider.

- Expressiveness: We investigate the languages definable in these logics.
- Satisfiability and model checking: The complexity of satisfiability and model checking for these logics are studied.

The title of the thesis comes from the observation that the quantifiers we consider, in the presence of a linear order, can only define regular languages. There are quantifiers like the unary counting quantifiers which can define nonregular languages.

In the first part of our work, we show that LTL extended with modulo counting/ group operators (LTLgrp) and FO[<] extended with modulo counting/group quantifiers (FOgrp[<]), both accept the same set of languages. We then go on to show that the satisfiability and model checking for LTLgrp is space-complete. We also look at satisfiability of various fragments of this logic. Then we show that the two variable fragment of FOgrp[<] is Expspacecomplete. We also analyse certain important sublogics.

In the second part of our work, we study first order logic with a linear order and the arithmetic predicate, +. We first show that the two variable fragment of FMod[<, +] is undecidable. Then we show that over a unary alphabet satisfiability of FMod[<, +] is 2Expspace. Finally we investigate the expressive power of M[<, +], where M is a set of monoid quantifiers. We show, using the concept of a neutral letter, that the class of neutral letter languages definable in M[<, +] is equivalent to those definable in M[<]. Using the above claim, we are able to show that the logics M1[<, +] is different from



- $M2[<, +]$, if the set of monoid quantifiers M_1 and M_2 are different. This lets us answer a conjecture of Roy and Straubing that $FO[<, +]$ and $\text{mod}[<, +]$ are incomparable. We also show that given a regular language L , it is decidable whether L is definable in $\text{mod}[<, +]$ or not.

Publications

Accepted (Conference)

1. Kamal Lodaya and A.V. Sreejith. LTL can be more succinct. In Proc. 8th ATVA, Singapore, volume 6252 of LNCS, pages 245–258, 2010.
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Accepted (Journal)

1. V. Sreejith. Expressive completeness for ltl with modulo counting and group quantifiers. Electronic Notes in Theoretical Computer Science, 278:201–214, 2011.

Submitted

1. Arvind, S. Raja and A. V. Sreejith. On Lower Bounds for Multiplicative Circuits and Linear Circuits in Noncommutative Domains In International Computer Science Symposium in Russia (CSR), 2014



Name : **Surendra Kumar Sharma**
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Title : Development of Compact Pulsed Power System and Study its Performance

Abstract

Nowadays, compact pulsed power technology that is robust and repetitive is driven by size, weight and volume constraints in recent times. In both the military and commercial applications, there is an overwhelming need to provide more and more capability in ever smaller and lighter packages. Certain applications require technology that can be deployed in smaller volume under stressful environments. The need for higher energy densities, power densities and efficiency is the driving force in this field. Remarkable advances in high energy density materials for capacitor development and new solid-state high power devices have enabled pulsed power systems to achieve reduction in size and weight. The research issues are still open on studying and utilizing new materials-dielectrics, insulators, metals, and interface in the design of sub-systems of the compact pulsed power systems. This development requires combined efforts at three levels: efficient and robust devices at component levels, novel circuits and architecture at the system level, and effective technique to deliver fast pulses at the application levels. Fundamental studies on compact pulse forming lines with high dielectric constant ceramics and alternative engineering topologies are investigated in the thesis. The research focus was on the studies on development of compact pulse forming lines using composite mixture of high dielectric constant ceramics such as barium titanate, and also investigating new engineering topologies using helical inner conductor to reduce the size of the pulse forming line that is used as intermediate energy storage in pulsed power system. This thesis describes the development of compact pulsed power system and its performance. The transmission line characteristics of the pulse forming line, which generates longer duration rectangular pulses, is also investigated and a novel technique for fast repetitive double pulse generation with very short inter pulse interval is also described.

Publications

1. "Compact pulsed power driver for double pulse effect studies in nanosecond laser ablation" Surender Kumar Sharma, P. Deb, R. Kumar, Archana Sharma and A. Shyam IEEE Transaction on Plasma Sciences, Volume 41, Issue 10, 2609 (2013)
2. "Fast double pulse system using the transmission line characterises of the pulse forming line" Surender Kumar Sharma, P. Deb, Archana Sharma and A. Shyam Review of Scientific Instruments, Volume 83, 115108 (2012)
3. "Compact helical pulse forming line for longer duration rectangular pulse generation" Surender Kumar Sharma, P. Deb, Archana Sharma, R. Shukla, T. Prabakaran, B. Adhikary and A. Shyam Review of Scientific Instruments, Volume 83, 066103 (2012)
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Name : **Aishwarya Soumitra Kar**
Enrolment No. : CHEM01200604017
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Speciation of Actinides and Lanthanides: Spectroscopic and Modeling Studies

Abstract

The depletion of fossil fuels based energy sources, viz., coal, oil and gas has envisaged nuclear energy to contribute significantly to the total electricity consumption in the coming years. However, the harnessing of nuclear energy as a viable major alternative to the other major energy sources would bring in the challenge of maintaining the growing nuclear wastes in the confines of their repositories, so that the future generations are not adversely affected by the radiations emitted by the actinides and long lived fission products. Although the radionuclide release from the repository to biosphere is expected to be prevented by multi barrier system, radionuclides may diffuse out of the glass matrix due to their decay heat, corrosion of canisters and/or natural calamities such as earth quakes, volcanic eruptions, followed by their dispersion and dissolution, which can ultimately lead to their release in biosphere. Therefore, it is imperative to have detailed knowledge about the migration of radionuclides in the aquatic environment which is significantly influenced by various organic and inorganic ligands present in the surrounding media. Humic acid (HA) and small complexing anions are prevalent in aquatic systems and hence their complexation with actinides and their influence on actinide sorption has been investigated in this thesis.

For complexation studies, Eu(III), the rare earth element having good fluorescence yield, has been used as an analogue of trivalent actinides to study the complexation of Eu(III) by different carboxylates, namely, alpha hydroxyisobutyric acid (HIBA), succinic acid, phthalic acid, mandelic acid and HA using time resolved fluorescence spectroscopy (TRFS) and the stability constant and stoichiometry of the Eu(III)- carboxylate complexes has been deduced.

In the studies pertaining to sorption, four different systems have been investigated.

- a) The effect of pH, ionic strength, HA concentration and order of addition of curium and humic acid on curium sorption by silica colloids has been studied. Linear additive model qualitatively reproduced the profile of the Cm(III) sorption by silica in presence of HA.
- b) Sorption of Eu(III) by silica and the effect of HIBA has been studied by batch sorption as well as TRFS. The speciation calculations of Eu(III) using MINTQA2 and the surface complexation modeling (SCM) of the binary and ternary systems using FITEQL4.0 has been carried out. The SCM has been validated using TRFS. Similar studies were performed with Cm(III) in order to demonstrate the differences, if any, between europium and curium with regard to sorption.
- c) Sorption of neptunium on hematite colloids has been studied under aerobic and anaerobic conditions at varying pH in absence and presence of HA. The stability constant of Np(V)-humate complex was determined by solvent extraction method. Under anaerobic conditions Np(IV) sorption on hematite was studied and drastic difference in sorption behavior were observed in aerobic and anaerobic conditions.
- d) Sorption of U(VI) on silica surface was investigated as function of pH, ionic strength, and U(VI) concentration by employing batch sorption experiments and SCM. The effect of complexing anions viz., carbonate and citrate on U(VI) sorption was also studied. SCM and TRFS were satisfactorily able to explain the sorption phenomena in all the systems.

The present work is a small step towards understanding the migration behavior of actinides and long lived fission products in the geosphere, which is a frontier area of research by the radiochemists



worldwide. With the availability of intense synchrotron sources and laser based spectroscopic instruments, the molecular structure of the actinides can be obtained, which in turn would help in validating the models proposed to predict the migration pathways of these long lived radionuclides in the geosphere upon their release from the deep geological repository.

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Symposium

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Name : **Naveen Kumar**
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Title : Experimental and Numerical Investigation of Mechanical Properties of Irradiated Ferritic/Martensitic Steel-T91 with Microstructure Evaluation

Abstract

The next generation fission and fusion reactors are expected to operate at a dose and temperature of above ~ 100 dpa and 500 OC respectively. The ferritic/martensitic steels are considered as candidate structural materials for the next generation reactors. The materials used for the core internal and external structural and functional materials undergo high energy particle irradiation. This particle irradiation leads to microstructural change by defect formation and its diffusion with respect to time. It has been found that the defect formation and other microstructural features formed due to irradiation manifest itself as change in macroscopic properties. The microstructural change and its macroscopic effects cover a wide range of length and time scale. In order to understand this wide scale phenomenon new methodology was developed by nuclear materials community known as Multi-scale Material Modeling (MMM).

In view of this, the main objective of the present work was to develop a methodology to predict the mechanical property change due to irradiation. As a first step, the nanoindentation experiment is carried out on argon ion irradiated samples to find the hardness change due to irradiation. The hardness extracted from nano indentation is correlated with yield strength, so, quantitative prediction of yield stress was made and satisfactory results are obtained. The material property changes due to irradiation were found to be due to nano scale defects formed such as void/bubbles/loops/precipitates as observed from microstructure characterization using transmission electron microscopy. The observed defects size and approximate density were quantified. The effect of these defects and their interaction with dislocations in matrix as well as at grain boundaries were studied using molecular dynamics (MD) and dislocation dynamics (DD) simulations. The MD and DD simulations were carried out on model materials such as pure Fe, Fe-10%Cr. It was found that the stress required for the dislocation to overcome the defects increases with increase in the defect diameter. It was also found that the voids are stronger obstacles to the dislocation motion than that of bubbles. At twist grain boundaries the defects obstruct the motion of network dislocation structure which increases the resistance for the grain boundary sliding. The helium gas atoms produced due to transmutation reaction in structural materials was found to have detrimental effect on the mechanical properties of the materials. In order to understand the effect of helium on the dislocation motion, MD simulations were carried out with helium in the matrix.

Effect of temperature and helium concentration was also investigated. It was found that the helium in the interstitial position have high resistance for the dislocation motion than that of substitutional one. MD simulation of nanoindentation was carried out to study the effect of defects on load displacement curves and dislocation evolution on different slip planes. It was observed that the distributed vacancies act as stronger obstacles to dislocations than loops. It was also found that the $\{123\}$ planes are equally active as that of $\{110\}$ family planes where $\{112\}$ comparatively least active. The outputs of MD simulation friction stress and obstacle resistance are used in DD simulations to estimate the yield strength/flow strength (YS/FS). It is found that the MD and DD methodology qualitatively predicts the change in mechanical property such as (YS/FS) determined from experiments.



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6. "Molecular dynamics simulation of edge dislocation motion in Fe-10%Cr model alloy with substitutional or interstitial He", N. Naveen Kumar, P.V. Durgaprasad, B.K. Dutta, G.K. Dey, ICCMS-12, Indian Institute of Technology, Hyderabad, 9-12 December, 2012.



Name : **Narender Kumar Goel**
Enrolment No. : CHEM01200804005
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Study of Radiation Induced Polymerization of Quaternary Ammonium Based Monomers for Biomedical and Environmental Applications

Abstract

Quaternary ammonium compound (QACs) have a broad spectrum of antimicrobial activity against both gram-positive and gram-negative bacteria. As compared with small molecule antimicrobial agents, polymeric antimicrobials have advantages in terms of being nonvolatile, chemically stable, long-term antimicrobial activity, and hard to permeate through the skin. Such materials can therefore in principle be attached to substrates like cotton via covalent bonding to produce biomaterials. Radiation grafting methods offer clean way of grafting (attaching) such monomers to polymers like cotton. The study reported in the thesis is aimed at investigating the polymerization and grafting behavior of derivatives of QACs, characterization of the resulting end products and evaluating them for the desired characteristics. The results showed that due to high reactivity of MAETC monomer in aqueous solution, homopolymerization was predominant over graft copolymerization. This thesis reports results from the research work towards radiation polymerization and/ or radiation induced grafting behavior of derivatives of QACs and their evaluation for health care and environmental applications. Efforts have been made to acquire new insights in obtaining the well characterized grafted and / or copolymerized QACs using radiation techniques. The results have been interpreted in terms of their antibacterial and dye uptake studies for healthcare and environmental applications.

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6. N. K. Goel, V. Kumar, Y. K. Bhardwaj, S. Sabharwal, Radiation induced co-grafting of Acryloyloxyethyltrimethylammonium chloride (AETC) and 2-Hydroxyethylmethacrylate (HEMA) onto cotton threads: optimization and characterization. "Trombay symposium on Radiation and Photochemistry" (TSRP-2008), 7-11 January 2008, YASHADA, Pune, India
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Presentation

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Best Poster Award

1. N. K. Goel, V. Kumar, Y. K. Bhardwaj, S. Sabharwal, Radiation synthesized stimuli-responsive HEMA-co-MAETC hydrogels, RC-05, APSRC-TSRP-2010, Sept 14-17, 2010, Lonavala, India.
2. N. K. Goel, V. Kumar, Y. K. Bhardwaj, and S. Sabharwal. Radiation induced co-grafting of Acryloyloxyethyltrimethylammonium chloride (AETC) and 2-Hydroxyethylmethacrylate (HEMA) onto cotton threads: optimization and characterization. "Trombay symposium on Radiation and Photochemistry" (TSRP-2008), 7-11 January 2008, YASHADA, Pune, India
3. N. K. Goel, V. Kumar, Y. K. Bhardwaj, K. A. Dubey, C. V. Chaudhari, S. Sabharwal, Antibacterial cotton fabric prepared by radiation grafting technique. "An international conference on Frontiers of Radiation and Photochemistry" 8-11 February 2007, Mahatma Gandhi University, Kottayam, Kerala, India



Name : **Kshitish Kumar Barada**
Enrolment No. : PHYS06200704009
Constituent Institute : Institute for Plasma Research, Gandhinagar
Title : Study of Wave Propagation and Potential Structures in an Expanding Helicon Plasma

Abstract

Diverging magnetic fields are found naturally in universe including our magnetosphere and in solar coronal funnels. Diverging magnetic fields are used in expanding plasmas to accelerate particles by electric fields produced by localized potential structures, called double layer, formed self consistently inside the plasma. Acceleration of charged particles in low temperature plasmas is of interest to surface function modification as well as to development of electrostatic thrusters. This thesis devotes its study to find the role of diverging magnetic fields in helicon source operation and self consistent potential structure formation in bulk of plasma. A geometrically expanding (small diameter source attached to a bigger diameter expansion chamber) linear helicon device along with various diagnostics is designed and built with a diverging magnetic field. The helicon plasma produced with an $m = +1$ half helical antenna powered by a 2.5 kW RF power source at 13.56 MHz is characterized. Mode transitions are observed and mode structures are studied at low magnetic fields (<100 G). Though a monotonic increase in density with magnetic field is expected for helicon plasma, multiple density peaks are observed for the first time for field variations at low magnetic fields and are explained on the basis of oblique resonance of helicon waves in a bounded geometry for the first time. Characterization on both sides of the antenna at low magnetic fields revealed the role of left circularly polarized waves in electron cyclotron absorption in bounded plasmas. Changing the magnetic field topology at low magnetic fields, it is found that diverging magnetic fields near antenna can increase the efficiency of the source as high as 80 % from the zero field case. With a magnetic field ~ 100 G near the source and ~ 10 G at the end of the expansion chamber, density peaks on axis are observed nearly two wavelengths away from the antenna where the field is ~ 35 G. Helicon wave phase measurements show that the wave does not propagate in the source region owing to the density cut-off of the wave but starts to propagate in the downstream for lower densities and magnetic fields. Finally, diverging magnetic fields and their gradient near the geometrical expansion location are varied to create strong potential structures along the magnetic field direction. The very first direct observation of multiple potential structures of varying strengths in current free plasmas is presented in this thesis.

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7. Kshitish K. Barada, P. K. Chattopadhyay, J. Ghosh, D. Sharma, and Y. C. Saxena. "The downstream density peak in low magnetic field helicon discharge" to be submitted.



Name : **Yeshpal Singh Rana**
Enrolment No. : PHYS01200704022
Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Theoretical Studies on Noise Techniques for Measuring Physics Parameters of Accelerator Driven Systems

Abstract

This thesis describes theoretical studies on the development of reactor noise methods for measuring sub-criticality of Accelerator Driven Systems (ADS). The principal difference between reactor noise in ADS and traditional reactors lies in the characteristics of the external source. There are reasons to believe that the accelerator produced neutron source cannot be assumed to be a Poisson process. As a consequence, the commonly used approaches in traditional reactor noise theory such as the Kolmogorov forward equation and the Bartlett formula are not applicable to the study of reactor noise in ADS. In view of this, a new theory of reactor noise in ADS considering periodically pulsed source and its non-Poisson character was developed earlier in BARC. The theory has been further developed in the thesis to treat the possibility of correlations between different source pulses, pulses of finite widths and delayed neutrons. Formulae for various noise descriptors such as Rossi alpha, Feynman alpha and power spectral density have been obtained. For the more general case of correlated non-Poisson pulsed sources with finite pulse width including delayed neutrons, we have developed the Langevin approach to obtain the PSD of the reactor noise in ADS. Experimental studies are planned in the Purnima sub-critical facility at BARC to study pulsed neutron and noise methods for measuring the sub-critical reactivity of ADS and to interpret the results in the light of the above theory. We have developed a few group diffusion theory based analogue Monte Carlo code for simulating the proposed experimental set-up. The simulator incorporates delayed neutron effects and dead time effects.

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5. Rana Y. S., Singh, Arun and Degweker, S. B. (2013), "Diffusion Theory Based Analogue Monte Carlo for Simulating Noise Experiments in sub-critical Systems," Nucl. Sci. Eng., 174, 245



Name : **Sushil Kumar Singh**
Enrolment No. : PHYS06200704019
Constituent Institute : Institute for Plasma Research, Gandhinagar
Title : Observation and Theory of Electron Temperature Gradient
Turbulence in Laboratory Plasma

Abstract

We present the experimental demonstration and theoretical model of Electron Temperature Gradient (ETG) turbulence in the finite beta laboratory plasma of Large Volume Plasma Device (LVPD). In magnetized plasma, the confinement problem starts with particle and thermal transport which becomes anomalous in nature due to small scale micro-instabilities. Recent numerical and experimental results reveal that ETG turbulence is more likely responsible for anomalous transport of plasma. The small scale nature of ETG mode inhibits its direct measurement in fusion devices whereas the basic plasma devices (linear and toroidal) provide conditions suitable to bring the scale length of the mode to measurable regime but faces problems because of the presence of ionizing hot and non-thermal electrons due to filamentary and other sources. The removal of unutilized primary ionizing and nonthermal electrons and control of radial gradient scale length in electron temperature are all achieved by placing a large Electron Energy Filter (EEF) in the middle of the LVPD. The EEF divides LVPD plasma region in source, filter and target plasma.

The electromagnetic ETG instability is investigated in the core plasma of the target region. We have established the turbulence by measuring the fluctuations (density, magnetic, temperature and potential), power-spectra, correlation, phase angle, propagation, wavenumber-frequency spectrum and beta scaling in suitable equilibrium plasma conditions for two EEF configurations, one for excitation and other of conformation of the ETG mode. The observed turbulence is characterized by broadband spectra in the lower hybrid range of frequencies following the power law. In the diagnostic, an electronically compensated Langmuir probe technique has been developed for accurate measurement of electron temperature and its fluctuations which are crucial parameters for turbulence study. Moreover, the experiment is performed for nonlinear coherent structures on a cross-field plane of core plasma in the background of ETG turbulence. The structures are determined from the conditional averaging technique of floating potential fluctuations taken by a poloidally separated array of Langmuir probes, moved to different radial locations with respect to reference probe. The experimental results will brief on size, lifetime, time evolution characteristic and nature of the observed structures.

The linear and nonlinear theory of coupled Whistler-Electron Temperature Gradient (WETG) mode is developed using two-fluid model applicable for LVPD plasma. The role of parallel and perpendicular magnetic field perturbations, non-adiabatic ion response and electron collisions are considered in the derived dispersion relations. The compared experimental and numerical results consisting of fluctuations level, frequency, correlation properties, phase velocity, mode characteristic and beta scaling of all fluctuation amplitudes are found in good agreement in accordance with electromagnetic ETG turbulence.

In addition to linear response, a theoretical model for secondary instabilities for long scale mode generation in the background of electromagnetic ETG turbulence is obtained using nonlinear fluid equations. The dispersion relation for zonal flows and streamers are obtained using the standard wave kinetic formalism. In the numerical results, zonal flows, zonal magnetic fields, electromagnetic streamers and pure magnetic streamers are shown to get excited by host turbulence. The interpretation of results obtained for nonlinear modes has also been discussed.



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3. Investigations on ETG turbulence in finite beta plasma of LVPD , S. K. Singh, L. M. Awasthi, S. K. Mattoo, P. K. Srivastava, R. Singh, and P. K. Kaw Plasma Phys. Controlled Fusion 54, 124015 (2012).
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6. Plasma Response to Electron Energy Filter in LVPD, nA. K. Sanyasi, L. M. Awasthi, S. K. Mattoo, P. K. Srivastava, S. K. Singh, R. Singh and P. K. Kaw Phys. Plasmas 20, 122113 (2013).
7. Investigations of Nonlinear Structures in Large Volume Plasma Device, S. K. Singh, L. M. Awasthi, S. K. Mattoo, R. Jha, P. K. Srivastava, R. Singh and P. K. Kaw (Accepted for publication in AIP proceeding).
8. Electromagnetic Secondary Instabilities of Coupled Whistler-ETG Turbulence, S. K. Singh, Rameswar Singh, L. M. Awasthi, R. Singh and P. K. Kaw IPR/RR-604/2013, (To be submitted in Physics of Plasma).
9. A 5 kA Pulsed Power Supply for large EEF solenoid in LVPD, P. K. Srivastava, S. K. Singh, L. M. Awasthi and S. K. Mattoo (To be submitted).

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1. Electromagnetic Secondary Instability of Whistler-Electron Temperature Gradient Turbulence in Finite Beta Plasma, S. K. Singh, Rameswar Singh, L. M. Awasthi, R. Singh and P. K. Kaw Sokendai Asian Winter School and Toki Lectures on Simulation Science, 10-13 December 2013 at NIFS, Toki, Japan.
2. Observation of Electromagnetic Turbulence in the Energetic Electron Belt region of LVPD Plasma, A. K. Sanyasi, L. M. Awasthi, S. K. Mattoo, P. K. Srivastava, S. K. Singh, R. Singh and P. K. Kaw 13th IAEA Technical Meeting on Energetic Particles in Magnetic Confinement Systems, 17-20 September 2013 at Beijing, China.
3. Experimental Observation of Coherent Structure in Finite Beta Plasma, S. K. Singh, L. M. Awasthi, S. K. Mattoo, R. Jha, P. K. Srivastava, R. Singh and P. K. Kaw The 6th ITER International School on RF Heating and Current Drive in ITER, 02-06 December 2012 at Ahmedabad, India.
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5. Investigations of Nonlinear Structures in Large Volume Plasma Device, S. K. Singh, L. M. Awasthi, S. K. Mattoo, R. Jha, P. K. Srivastava, R. Singh and P. K. Kaw International Conference on Complex Processes in Plasma and Nonlinear Dynamical System (ICCPNDS-2012), 6-9 November 2012 at Gandhinagar, India.
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7. Revisiting Plasma Hysteresis with an Electronically Compensated Langmuir Probe, P. K. Srivastava, S. K. Singh, L. M. Awasthi and S. K. Mattoo 8th General Scientific Assembly of the Asia Plasma and Fusion Association, 1-4 November 2011 at Guilin, China.
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Name : **Deepak Sangwan**
Enrolment No. : PHYS06200704013
Constituent Institute : Institute for Plasma Research, Gandhinagar
Title : Studies of Plasma Flows in Scrape-Off Layer Plasma of Aditya Tokamak

Abstract

In this thesis, the scrape-off layer (SOL) plasma flow studies are carried out in ADITYA tokamak. Measurements are carried out at different operating parameters and different spatical locations. The main motivation is to present a comprehensive studies of plasma flow. Plasma flows, construct the possible flow pattern, and determine possible cause of the plasma flow. Plasma flows in the SOL region have been measured and studied in most of the tokamaks. It is now well recognized that SOL plasmas flows play crucial role in the impurity control, L/H transition and global confinement of tokamak plasma. This happens because the SOL is the inter-mediating layer between main plasma and the material surface and all the plasma surface interaction takes place in this region.

In ADITYA contact of the plasma with the limiter is only in the limited poloidal region, not in the whole poloidal plane. This makes the SOL of ADITYA special. The specially is observed in terms of simultaneous existence of long and short connection lengths L_{\parallel} in the SOL plasma. The effects of long and short L_{\parallel} observed in terms of different density decay lengths at the top of the plasma and at the outboard locations, for the measurements carried out in low toroidal magnetic field $BT \sim 0.2$ T and low plasma current $I_p \sim 25$ kA. The parallel flow Mach number M measurements are carried out by Mach probe. The measured M shows the presence of the contributions from the Pfirsch-Schuler (PS) flow, $E \times B$ drift and sink action of the limiter. The parallel flow direction is in the side of limiter and the ploidal flow towards the plasma limiter contact point.

To ascertain the effect of the extra particle source on the different SOL properties including flows, experiments with a small puff of working gas has been carried out in high $BT \sim 0.75$ and high $I_p \sim 80$ kA. Along with the role of the PS flow, $E \times B$ shows the coupling between turbulence, and mean plasma flows, as another possible driving mechanism for SOL flows. It is also observed in different tokamaks. This coupling is washed out during the gas puff. The importance of M in controlling the particle flux is also seen. The M is observed to increase with gas puff at two different locations, and show the change in the flow direction at the outboard midplane location. The decrease in the electron temperature and floating potential fluctuations are seen with the gas puff. On the other hand, the fluctuations in ion saturation current remain unchanged.

In above experiments, we have seen that in ADITYA, both transport driven and drift driven flows components are present. Here, the transport driven, and drift driven flow components are independent, and dependent on the BT and IP directions, respectively. We have carried out experiments in all four direction combinations of BT and IP, to separate out the two flow components. The two flow components are indentified by using $M1, 2 = M_{tr} \pm M_{dr}$, where \pm is for the two direction combination of BT and IP, and M_{tr} are the transport and drift driven Mach numbers, respectively. The $E \times B$ drift, and PS flows are main causes behind the drift driven component, and ballooning type transport, and sink action of limiter are two major causes behind the transport driven flow component. The presence of ballooning transport is verified by the polodial asymmetry in the radial particle flux and plasma density.



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1. Deepak Sangwan, Ratneshwar Jha, Juana Brotankova, and M. V. Gopalkrishna “Plasma flows in scrape-off layer of Aditya tokamak”, *Phys. Plasma* (19), 092507 (2012).]
2. Deepak Sangwan, Ratneshwar Jha, Juana Brotankova, and M. V. Gopalkrishna “Modification Plasma flows with gas puff in the scrape-off layer of ADITYA tokamak”, *Phys. Plasmas* (Accepted).
3. Deepak Sangwan, Ratneshwar Jha, Juana Brotankova, and M. V. Gopalkrishna “Identification of Transport Driven SOL flow in two Different Helicities in ADITYA Tokamak”, (under preparation)



Name : **A. Jasmin Sudha**
Enrolment No. : ENGG02200704002
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Mathematical Modelling of Fuel Melting and Relocation During a Severe Accident in a FBR

Abstract

Fast Breeder Reactors (FBRs) are provided with redundant and diverse plant protection systems with a very low failure probability ($<10^{-6}$ /reactor year), thus making Core Disruptive Accident (CDA), a Beyond Design Basis Event (BDBE). Nevertheless, safety analysis is carried out even for such events in order to mitigate their consequences by providing engineered safeguards such as the in-vessel core catcher. During a CDA, a significant fraction of the hot molten fuel moves downwards and gets relocated to the core catcher. The core catcher design requires a priori knowledge of core-melt relocation time which is the time taken for the molten fuel to reach the lower plenum from the active core region. This is because of the fact that the decay heat contained in the fission products of the core-melt is a strong function of time.

Therefore the initial thermal load on the core catcher is primarily dictated by the core melt relocation time. This research work aims at determining the upper and lower bounds for core melt relocation time for postulated accident conditions of Protected Loss of Heat Sink (PLOHS) accident and Unprotected Loss of Flow Accident (ULOFA) respectively. The natural convection setting in the cold sodium plenum which can influence this time estimate is also studied with a view to prescribe proper boundary condition for the grid plate bottom following a ULOFA. Finally, a new multi layer core catcher capable of handling the debris generated from a whole core melt down accident is proposed.

In the first part of the research work, Nusselt number correlations are developed for natural convection setting in liquid sodium filled cylindrical enclosure with particular emphasis on the lower sodium plenum of the reactor main vessel. For estimating the time taken for grid plate melt-through in case of ULOFA, a computer code HEATRAN-1 is developed which solves transient nonlinear heat conduction equation including phase change. The code is a finite difference code based on enthalpy formulation and incorporates Voller's improved algorithm for tracking the melt-front. In case of PLOHS, molten material relocation is analyzed starting from the active core region, sequentially moving through the lower axial blanket region, lower fission gas plenum, tail piece of subassembly with flow entry nozzles and honeycomb structures for flow zoning, discriminator at the foot of the subassembly and the grid plate. Each region is approximated as a porous body with effective thermophysical properties and heat conduction analysis is carried out to estimate the core-melt relocation time. In the final part of research work, a new multi layer core catcher is conceptualized which essentially consists of a top refractory layer, a middle delay bed and a base layer. The thickness of the intermediate delay bed is optimized to limit the temperature at the base layer within design safety limits by heat transfer analysis.

Keywords: Phase change heat transfer, enthalpy method, core melt down, fast reactor safety, grid plate melting, Conjugate heat transfer, Nusselt number correlation, multi layered core catcher



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4. An Enthalpy Method to Predict Core-Melt Propagation during Severe Accident in a Fast Reactor, A.Jasmin Sudha and K.Velusamy, ASME-ISHMT Conf. on HMT, Jan 2010, Mumbai



Name : **Ashit Krishna Pattanaik**
Enrolment No. : CHEM02200704004
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Experimental Investigations on the Phase Diagram and Thermodynamic Properties of U-Sn System

Abstract

Phase diagram and thermodynamic properties of U-Sn system are useful for fast reactor technology. The system has five intermetallic compounds. All the alloys used in the study were prepared by a tri-arc furnace, annealed and characterized before use. Phase diagram study of the above system was studied out using spot technique developed in house. In this method, a metal or an alloy is taken in an inert ceramic cup in a Knudsen cell (K-Cell) and heated by a non-contact means (RF Generator) in vacuum. For an alloy, the appearance of the first spot similar to the image formed by a broken mirror corresponds to the solidus temperature. These tiny broken spots coalesce to form a single dark spot which corresponds to the liquidus temperature. So both the solidus and liquidus temperatures can be determined. The technique was used to find out the peritectic melting temperatures of USn, USn₂, U₃Sn₇ and USn₃ in the U-Sn system.

The Gibbs energies of formation of USn₃, U₃Sn₇, USn₂ and USn in the temperature range 682-905 K were determined using molten salt galvanic cell emf measurements. In this method eutectic salt of LiCl-KCl loaded with UCl₃ was used as the electrolyte. Before loading the salt, the concentration of uranium in the salt was determined using Davis-Gray method. The Gibbs energies of formation of U₃Sn₇, USn₂ and USn were reported for the first time. High temperature aluminium solution calorimeter was used to determine the enthalpy of formation of USn₃ at 298.15 K.

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2. Gibbs free energy formation of U₃Sn₇ by galvanic cell measurement, **A. K. Pattanaik**, R. Kandan, K. Ananthasivan, B. Prabhakara Reddy, K. Nagarajan, P. R. Vasudeva Rao, Oral presentation, Chemistry Research Scholar's Meet, Indira Gandhi Centre for Atomic Research, Kalpakkam, India, July 14-15, 2011.
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Workshop

1. Attended a workshop on "Metallurgy for Non-Metallurgist", Organized by IIM-Chennai Chapter, Chennai, March 3-4 2009.



Name : **Srijit Bhattacharjee**
Enrolment No. : PHYS05200704007
Constituent Institute : Saha Institute of Nuclear Physics, Kolkata
Title : Quantum Infrared Instabilities of Gauge and Gravity Coupled Higgs Fields

Abstract

In my doctoral work I have studied quantum vacuum structure of theories where gauge bosons and gravitons are coupled to Higgs fields. To study the perturbative vacuum of a quantum field theory, effective potential plays a very important role since it includes radiative corrections over the tree level potential. It can be computed using a semi-classical expansion in number of loops or alternatively in powers of Planck constant. For massless case this one-loop effective potential is known to be as Coleman-Weinberg potential. However, being an off-shell quantity it is naturally plagued by gauge ambiguities although it has wide applications in different area of physics. I have studied this mechanism to make it free of gauge dependencies. This was done rewriting abelian and non-abelian gauge theories in terms of manifestly gauge-inert variables. It was shown that massless scalar electrodynamics gives a unique scalar to vector mass ratio. However, one can still ask about reparametrization invariance of the effective potential which was taken care of by recombining the gauge-free theory with the Vilkovisky-DeWitt geometric method. We have also successfully able to rewrite $SU(2) \times U(1)$ theory in terms of completely gauge inert variables and generated a CW potential without any Higgs self coupling therefore avoiding the question of naturalness!

The gravitational analogue of CW potential is more interesting. Gravity being a non-linear theory develops additional instability in the infrared limit when coupled to Higgs fields. The theory is quantized using functional integral technique with the background space time is taken to be Minkowskian (or Euclidean). Computation of the one-loop effective potential for this theory with a constant scalar background develops an imaginary term. This is traced to the appearance of a tachyonic pole in the graviton propagator. This instability is analogous to the finite temperature infrared instability of a gas of gravitons coupled to fermions found by Gross et. al., even though it already exists at zero temperature; it is thus reminiscent of the Jeans instability thought to be at the heart of structure formation in the early Universe.

I next looked into another theory where scalar fields are coupled with some higher derivative terms in Gravity. The source of such couplings had a different motivation. These had arisen to construct gauge invariant coupling of different fields with torsion. Here also an imaginary term is generated in the one-loop effective potential indicating vacuum instability. I have also studied behaviour of gravitational wave in Minkowski background in presence of such interactions. This new interaction gives rise to a modulation of the amplitude of the gravitational wave. The very nature of modulation i.e. whether it is attenuated or amplified depends upon the nature of interacting scalar field which can be either parity even or parity odd state. If such effects are present, they have implications for the Cosmic Microwave Background spectrum. They lead to non-zero cross-correlation in multipole moments C_l^{TB} and C_l^{TE} i.e., involving the parity-violating B-modes of the CMB spectrum.



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7. Gauge-free Electrodynamics, Parthasarathi Majumdar and Srijit Bhattacharjee, arXiv: 0903.4340, [hep-th].



Name : **Rakesh Kumar**
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Constituent Institute : Bhabha Atomic Research Centre, Mumbai
Title : Synthesis and Characterization of Membrane Supported Metal Nanoparticles

Abstract

Metal nanoparticles have interesting size-dependent properties that are significantly different from those of the corresponding bulk materials. The embedding of metal nanoparticles into membrane matrix can be potential solution to the manipulation and stabilization problems of nanoparticles. Polymer membranes embedded with metal nanoparticles are potentially useful for a number of technological applications.

This thesis describes the possibility of controlled formation of metal nanoparticles in ion exchange membranes. Silver and rhodium nanoparticles have been prepared in the matrix of Nafion-117, which is a cation exchange membrane, by *in situ* reduction of cationic metal ion precursor present in the membrane. The choice of ionic or non-ionic reductant dictated the size and spatial distribution of silver nanoparticles in the membrane matrix. Nafion with homogenously dispersed Ag nanoparticles has shown the enhanced diffusion mobility of slow moving counterions ions. Galvanic reactions of Hg^{+2} with Ag nanoparticles in the membrane have shown blue shift and decrease in the surface plasmon resonance absorption. This property can be used for the development of chemical sensor for Hg^{+2} ions. An anion-exchange polymeric inclusion membrane have been prepared by physical immobilization of liquid anion exchanger, Aliquat-336, in the matrix formed by plasticized cellulose triacetate (CTA). Changes in the properties (surface morphology, glass transition temperature, ion-exchange capacity, intrinsic diffusion property etc.) of the membrane due to compositional variation in the membrane have been studied. These membranes have been used to prepare homogenously dispersed gold nanoparticles from the anionic metal precursors. Repeated sequential cycles of loading and reduction of $AuCl_4^-$ ions in the membrane matrix have been carried out to increase the amount of gold nanoparticles in the membrane matrix. Self-diffusion mobility of iodide ions has increased after formation of the Au nanoparticles in membrane matrix.

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Name : **Sourav Mitra**
Enrolment No. : PHYS08200804002
Constituent Institute : Harish Chandra Research Institute, Allahabad
Title : Physics of Cosmological Reionization and Structure Formation in the Universe

Abstract

Using a semi-analytical reionization model, we study the observational constraints on reionization via a principal component analysis (PCA). We decompose the unknown function $N_{\text{ion}}(z)$, representing the number of photons in the IGM per baryon in collapsed objects, into its principal components and constrain it using three different data sets – the photoionization rates, the redshift distribution of Lyman Limit Systems and the CMBR angular power spectra using WMAP7 data. Using Markov Chain Monte Carlo methods, we find that all the quantities related to reionization can be severely constrained at $z < 6$ whereas a broad range of reionization histories at $z > 6$ are still permitted by the current data sets (Mitra et al. 2011). With the forthcoming PLANCK data on large-scale polarization, the $z > 6$ constraints will be improved considerably (Mitra et al. 2012).

One of the most crucial issues regarding the evolution of intergalactic medium (IGM) and cosmic reionization is the escape fraction, f_{esc} , of ionizing photons from high-redshift galaxies. This parameter remains poorly constrained in spite of the many theoretical and observational attempts made in past few years. We propose a novel, semi-empirical approach based on a simultaneous match of the most recently determined Luminosity Functions (LF) of galaxies in the redshift range $6 \leq z \leq 10$ with reionization models constrained by a large variety of experimental data (Mitra et al. 2013). From this procedure we obtain the evolution of the best-fit values of f_{esc} along with their $2\text{-}\sigma$ limits.

Reionization process could affect the determination of the cosmological parameters. So, we perform an analysis of the recent WMAP7 data considering physically motivated and viable reionization scenarios with the aim of assessing their effects on cosmological parameter determinations. The main novelties are: (i) the combination of CMB data with astrophysical results from quasar absorption line experiments; (ii) the joint variation of both the cosmological and astrophysical parameters. We find that the inclusion of a realistic, data-constrained reionization history in the analysis can induce appreciable changes in the cosmological parameter values deduced through a standard WMAP7 analysis (Pandolfi et al. 2011). We also try to investigate the possible effects on neutrino mass bound by considering our data-constrained reionization model and we find that, a more strict constraint on the neutrino masses can be achieved using this model.

Next, we derive an estimate of the rate of formation of dark matter haloes per unit volume as a function of the halo mass and redshift of formation. We develop a new prescription to calculate halo formation rate, using excursion set formalism but avoiding the assumption of scale invariance of halo destruction rate efficiency made by Sasaki. We compute the formation rate for the Press-Schechter and the Sheth-Tormen mass function and show that the formation rate computed in this manner is positive at all scales (Mitra et al. 2011) unlike the Sasaki prescription where one can get the unphysical results for the Sheth-Tormen mass function.

Final part of this thesis describes a method for constraining large scale HI bias using 21-cm signal from the post-reionization epoch. We investigate the nature of large scale HI bias and explore the possibility of constraining $b(k)$ using the Principal Component Analysis (PCA) on simulated data



(Guha Sarkar et al. 2012). We show that our method can be successfully implemented on future observational data sets to constrain $b(k, z)$ and x_{HI} and thereby enhance our understanding of the low redshift Universe.

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2. Mitra, Sourav; Kulkarni, Girish; Bagla, J. S.; Yadav, Jaswant K., Formation rates of Dark Matter Haloes, BASI 39, 563, (2011), arXiv:1103.5828
3. Mitra, Sourav; Choudhury, T. Roy; Ferrara, Andrea, Joint quasar-cosmic microwave background constraints on reionization history, MNRAS 419, 1480, (2012), arXiv:1106.4034
4. Pandolfi, S.; Ferrara, A.; Choudhury, T. Roy; Melchiorri, A.; Mitra, Sourav, Data- constrained reionization and its effects on cosmological parameters, PhRvD 84, 123522, (2011), arXiv:1111.3570
5. Guha Sarkar, Tapomoy; Mitra, Sourav; Majumdar, Suman; Choudhury, Tirthankar Roy Constraining large scale HI bias using redshifted 21-cm signal from the post-reionization epoch, MNRAS 421, 3570, (2012), arXiv:1109.5552
6. Mitra, Sourav; Ferrara, Andrea; Choudhury, T. Roy, The escape fraction of ionizing photons from high redshift galaxies from data-constrained reionization models, MNRAS Letter, 428, L1, (2013), arXiv:1207.3803



Name : **Soubhadra Sen**
Enrolment No. : PHYS02200704006
Constituent Institute : Indira Gandhi Centre for Atomic Research, Kalpakkam
Title : Computational Modeling of the Migration of Radioactivity in a Porous Medium

Abstract

To meet the ever increasing demand of energy, we need to resort to the use of the nuclear energy. The high level radioactive waste from the fission products of the nuclear reactors are concentrated and then vitrified into a glass matrix. Then they are sealed in a container which is buried inside the earth surface at a depth of 500m or more. In case of an accidental breach of the container, the radioactive waste will come in contact with rock and the radionuclides will migrate through the pore water of the rock. This radioactivity buildup due to this migration needs a realistic modeling to assess the environmental and radiological impact.

There are two routes to address this problem. The first way is a deterministic modeling of the migration process. Here one assumes a neat geometry of the rock. The medium is assumed to be a combination of an infinite array of parallel fractures of equal width separating identical porous matrices. Now the migration in the porous matrix and along the fracture can be described by a set of coupled partial differential equations. To assess the solution reliably for longer times and larger distances, four efficient finite difference schemes namely the Crank- Nicolson, the Dufort-frankel, the 4-th order Crank-Nicolson and the Higher Order Compact schemes are used to solve these governing partial differential equations. These governing equations are also solved by a more accurate method, called the psuedospectral method. Here we use both the Chebyshev and the Legendre pseudospectral methods. A detailed comparison of the relative accuracies of these schemes and the ranges of their applicability are then indicated. These higher order finite difference methods together with the pseudospectral schemes provide an efficient algorithm package by which concentrations can be assessed reliably for longer distances like 500m.

The second route of modeling is via a probabilistic estimation. In this work, we developed a methodology where the better aspects of the deterministic and the probabilistic approaches are optimally coupled. Using the concept of random walk, we generate an effective migration length between the source and the observation point. The average width of the porous matrix sandwiched between two consecutive fractures is also estimated. Subsequent calculations are performed using the deterministic parallel fracture model. In these calculations, we replace the linear fracture length by an average migration length. The average width of the porous matrix is chosen parametrically from a range indicated by the probabilistic estimation. A comparison of the concentrations as calculated by the two approaches (deterministic and probabilistic) is provided. As expected, the nondeterministic model proves to more realistic and less conservative.

At the end of the thesis, we report a numerical experimentation based on the Crank-Nicolson scheme. Two variants of the method, one centered around the half integer time step and the another centering around an integer time step are averaged to get a new generalized variant of the scheme. This new one like the other two is also unconditionally stable for the diffusion problem. Moreover, this scheme indicates the onset of solution quite early. However, this new scheme does not provide a time step advantage. It promises a better accuracy for complicated flow problems. Further studies are required along this line to exploit the advantages that will stem from this variant of a classical method.



Publications

1. S. Sen and N. Mohankumar, "A computational strategy for radioactivity migration in a porous medium", Ann. Nucl. Energy 38(2011) 2470.
2. S. Sen and N. Mohankumar, "A note on higher order numerical schemes for radioactivity migration", Ann. Nucl. Energy 49 (2012) 227.
3. S. Sen and N. Mohankumar, "A random walk based methodology for the realistic estimation of radioactivity migration in a porous medium" Ann. Nucl. Energy 60 (2013) 202.
4. S. Sen and N. Mohankumar, "Migpore, a code package for the estimation of migration of radioactive species in a porous medium" Comput. Phys. Commun. 185 (2014) 302.



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Annex 5

**Titles of M.Tech,& M.Sc. (Engg.) theses for which
results were notified during April 1, 2013 to March 31, 2014**



**Titles of M.Tech. Theses for which results were notified
during April 1, 2013 to March 31, 2014**

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
1	Shri Somnath Jha	07.04.13	Seismic Margin Assessment of Shear Walls Considering Effect of Aspect Ratio
2	Ms. Sutanwi Lahiri	07.04.13	Technology Assessment of Atomic Vapour Laser Isotope Separation(AVLIS) Process
3	Shri Mahesh M.	07.04.13	Validation of 2-D Diffusion Theory for Accumulator and Its Application to Estimate Radon Flux and Diffusion Coefficient
4	Shri Harshit Tyagi	19.04.13	Study, Analysis and Prototype Demonstration of High Power Switching Topologies for Pulsed Power Modulator Applications
5	Shri Sujith P. K.	19.04.13	Life Predictions of Linking Pins of Natural Circulation Valve Test Setup of Upgraded APSARA Reactor
6	Shri Sulabh Gupta	29.04.13	Analysis of CVD Reactor for Silicon Production using CFD Code
7	Shri Venkatesh Kandalam	29.04.13	Hydrodynamic Study of Two Phase Flow in Wire Gauze Type Structured Packing using CFD
8	Ms. Sreeja Raj Menon	29.04.13	Computer Simulation on Radon Detection using Nuclear Track Detectors in Cylindrical Diffusion Chambers and Application of Cylindrical Dosimeter for Radon/Thoron Exhalation Measurement from Samples
9	Shri Shreesh Shauraya	20.05.13	Failure Diagnostics & Health Management of Pneumatic Control Valves
10	Shri Abdulhussain Amravatiwala	20.05.13	Design of Safety Critical System using FPGA
11	Shri Mayank Chaudhary	20.05.13	Remnant Life Assessment of Steam Generator Component: Secondary Super heaters



Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
12	Shri Satishkumar S.	20.05.13	Structural Design of Integrated Cold Trap
13	Shri Niranjan Diwan	20.05.13	Identification and Modeling of Different Electromagnetic Interference (EMI) Sources in Reactor Building for Improved EMI Assessment
14	Shri T. Teja Swaroop	20.05.13	Compliance Control of a Tele - Robot
15	Shri Praveen Kumar Srivastava	20.05.13	Effect of Process Parameters on Particle Size and Size Distribution of Thorium Powder Produced by Calciothermic Reduction
16	Shri Vipin Kumar Sharma	20.05.13	Analysis of Structures using Adaptive Pushover (Iterative Response Spectrum) Method
17	Shri Mabin Joseph Puthiakulangara	20.05.13	Statistical Analysis, Cryptanalysis and Efficient Study of eStream Profile-I Synchronous Stream Ciphers
18	Shri Vikrant Raizada	20.05.13	Modelling of Hot Extrusion Process for Inconel Alloy
19	Shri Sachin Gupta	20.05.13	Aberration Study and Design of Focussing Lens for Electron Beam Micro Welding Machine
20	Shri T. Chandra Kiran	20.05.13	Grid and Plant Interaction Simulation Study for PFBR
21	Shri Sreejith Sasidharan	20.05.13	Interactive Walkthrough and Interactive Fuel Handling Animation
22	Shri Nawaz Nazir Satvilkar	20.05.13	Design and Development of Controller for Capacitor Discharge Welding Machine
23	Ms. Rosy Sarkar	20.05.13	Investigation of Structural Integrity of Fuel Cladding under Normal & Extreme Loading Conditions
24	Shri Joel Jose	20.05.13	Design and Implementation of a Wireless Control System for a Remote Vehicle using TCP/IP Protocol



Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
25	Shri Pradeep Rautela	20.05.13	Design, Simulation and Implementation of Microprocessor Based Controller for Thyristor Converters Utilised for Simulating Power and Temperature Transients in an Experimental Facility
26	Shri Dubal Chaintanya Sadashiv	20.05.13	Development of Design Charts for External Pressure Design of Tubes Made of Titanium Alloy(IIT-7M)
27	Ms. Molly Mehra	20.05.13	Risk Cost Optimization for Safety Critical System of PFBR using Genetic Algorithm
28	Shri M. Chaitanya Reddy	28.05.13	Optimization of Rolling Schedules of Zircaloy-4 Sheet Products
29	Shri Rajesh Kumar Yadav	28.05.13	Strength Evaluation of RC Beams and Columns with Corroding Reinforcement
30	Shri Junaid Nisar	28.05.13	Preparation and Characterization of Glassy Carbon Catalyst Support
31	Shri Firoz Alam	28.05.13	Design, Analysis, and Testing of Hybrid Motor Having Improved Starting Performance
32	Shri Avimanyu Banerjee	28.05.13	Development of Risk Analysis Methodology for H ₂ S Based Heavy Water Plants
33	Ms. Kousiki Ghosh	05.06.13	Measurement and Analysis of Neutron Energy and Linear Energy Transfer Distribution in Pu Handling Facilities
34	Shri Rakesh A. R	06.06.13	Design of Containment for High Speed Rotating Disk Failure
35	Shri Deepak Kanse	13.06.13	Assessment of Suitability of Different Statistical Models to Predict the Strength of Graphite
36	Shri Mohamad Altaf	13.06.13	Determination of Residential Strength of Dynamically Loaded Structures Made up of Ferrite Steel, Based on Dynamic Fracture Mechanics Parameters
37	Shri Deepak Kumar Dewangan	13.06.13	Evaluation of Performance of RCC Shear Wall Using Non-Linear Model
38	Shri Prashant Dewan	13.06.13	SeismicBase Isolation of Mobile Hot Cell



Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
39	Shri Nirmal Das	01.07.13	Modeling of Data Communication Mechanism for PFBR Simulator
40	Shri Shirhatti Vijay Dhruva	01.07.13	Optimization of Reduction Process in Zirconium Sponge Production
41	Shri Abhishek Singh	01.07.13	Computational Fluid Dynamics Studies in Complex Flow Fields of Solvent Extractors
42	Shri Anindya Bhattacharyya	01.07.13	Design & Development of Control and Safety Logic System with Design Diversity for Evaporator in DFRP
43	Shri Vishnu Anand P.	01.07.13	Modeling and Simulation of Distillation Column for the Separation of TBP and n-Docane Mixture
44	Shri Subhramanyu Mohapatra	11.07.13	Analysis & Design of Digitally Controlled Variable Frequency Sine Wave Power Inverters, With Optimized Modulation Indices
45	Shri Vora Allarakha Yusuf	11.07.13	Stability Studies of Emulsion Based Extractant System for Recovery of Uranium from Dilute Waste Streams using Polymeric Surfactant
46	Shri Debasis Sinhamahapatra	11.07.13	Development of Methodology for Estimation of Low Energy Synchrotron and High Energy Bremsstrahlung Radiation Dose
47	Shri Jobby c. Johnson	11.07.13	Design of Distributed Control System for Hyper Redundant Robotic Applications Using CAN Protocol
48	Shri Tapan Kumar Sawarn	11.07.13	Investigation of the Ballooning and Deformation Behaviour with Associated Microstructural Changes of the Indian PHWR Fuel Cladding under Simulated LOCA Condition
49	Shri Saurav Sunil	13.07.13	Study on Influence of State of Stress on Delayed Hydride Cracking Behaviour of Zr-2.5Nb Alloy



Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
50	Shri Anupam Kumar Sinha	16.07.13	Theoretical Modeling, Numerical Simulation and Experimental Validation of Double Wedge Tuner Performance at Different Temperatures
51	Shri Priyabrata Jenamani	26.07.13	Speed Control of Induction Motor Using Variable Frequency with Sensorless Vector Control Method
52	Shri Raghavan Komanduri	26.07.13	Design and Development VMEbus Interface Controller (VIC) for Computer Based I & C Systems of Fast Reactors
53	Shri Dakinedi Durga Prasad	26.07.13	Estimation of Carbon-14 Emission Rates from Pressurized Heavy Water Reactors and Dose Assessment Using Dispersion Model
54	Shri Bipattaran Halder	26.07.13	Estimation of Uranium Concentration in Non-Standard Geometries using Gamma-ray Spectrometry
55	Shri Hitesh Mohanlal Kewlani	26.07.13	Development and Testing of Langmuir Probe Circuit for Online Measurement of Plasma Parameters in ECR Ion Source
56	Shri Niraj C. Deobhankar	26.07.13	Prediction and Residual Stresses in Pipe Welds using FEM and its Effect on Crack Driving Force
57	Shri Biswajit Kumar Kar	30.07.13	Establishing Corrosion Behaviour of Surface Worked Stainless Steel 304L and Reverting the Deleterious Effects
58	Shri Pradip Singh Nehra	01.08.13	Improving Resistance to Sensitization and Intergranular Corrosion of Alloy 600 for use in Nuclear Power Reactors
59	Shri D.D. Bhende	01.08.13	Evaluation of Fatigue Fracture Behaviour of VT-20 Titanium Alloy and its Weld
60	Shri Kiran V. Nagaraj	01.08.13	Establishing the Sensitization and Intergranular Corrosion Behavior of X-750 for use in Nitric Acid Environment
61	Shri Gurjap Singh	19.08.13	Mobile Robot Localization using Kinect RGB-D Sensor
62	Shri Gaurav Khullar	19.08.13	Vulnerability Analysis of Electronic Circuits for the Effect of High Power Microwave



Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
63	Shri Inderjit	19.08.13	Study and Modeling of Failure Mechanisms in CMOS Electronics and Accelerated Testing
64	Shri Gaikwad Girish Dwarkanath	20.08.13	Study on Application of Reverse Osmosis Techniques for Decontamination of Contaminated Portable Water
65	Shri Punna Rajasekhar	26.08.13	Study, Characterization and Performances Analysis of Switches and Routers in Switched Ethernet Networks for use in Real Time Systems of NPPs
66	Shri Shashank Singh Gaur	10.09.13	Development of Integrated Cryostat TL-OSL Studies of Doped Inorganic Phosphors, Biological Samples
67	Shri Sujeesh S.	12.09.13	Study of Bunsen Reaction at Elevated Temperatures and High Pressures
68	Shri Abhimanyu Chowdhury	19.09.13	Study, Simulation and Development of In-Situ Time Response Measurement System for RTDS
69	Shri Arunprasath V.	25.09.13	A System Identification Approach for On-Line Time Constant Computation of Thermocouples and Improvement of its Response Time by Bayesian Estimation
70	Shri Naveen Kumar	25.09.13	Simulation Studies on the Performance of Aerostatic Double Thrust Bearings of Cryogenic Turboexpander Rotor
71	Shri Ankit Kumar	26.09.13	Design & Development of Universal Signal Conditioning System on 12C Bus for Future FBRs
72	Shri Rajiv Kumar Yadav	26.09.13	Design and Implementation of Open Source Based HMI/SCADA System for Fast Reactor Fuel Cycle Facility (FRFCF)
73	Shri Pankaj Kumar Singh	10.10.13	Study of Iodine Spiking Following Reactor Shutdown in Indian PHWRs
74	Shri S. Krishna Aditya Yannam	22.10.13	Computational Investigation of Buoyant Flows in Inclined Differential Heated Cavities
75	Shri Malay Ghosh	22.10.13	Geochemical Modeling of Uranium Speciation in Subsurface Aquatic Environment of Chitradurga, Karnataka



Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
76	Shri Abhishek Chakrabarti	22.10.13	Fatigue Damage Characterization of Nickel Aluminium Bronze
77	Shri Ravi Kumar Gupta	22.10.13	Error Model and Accuracy Analysis of 6-DOF Parallel Manipulator
78	Shri Ritu Raj Bhati	22.10.13	Analysis and Testing of Frequency Control Module and Switching Network of RF System for Vertical Test Stand
79	Shri Raveendra K.	22.10.13	Modeling and Experimental Studies on Influence of Distributor Design in Fluidized Bed
80	Shri Mukesh Kumar Pal	22.10.13	Electromagnetic Design Studies of Low and Medium Beta Superconducting TEM-Class Resonators for 1 GeV Proton Linear Accelerator
81	Shri Ramesh Kumar	22.10.13	Evaluation of Thermal Stratification Induced Stress in Pipe and its Impact on Fatigue Design
82	Shri Abhishek Chatterjee	22.10.13	Electrical Characterization of Nitride Epitaxial Layers
83	Shri Shoubhik Chakraborty	22.10.13	Design and Development of FPGA Based Real Time RF Cavity Simulator
84	Shri Tirtha Mandal	22.10.13	Experimental Study of Fast Electrons from the Interaction of Ultra-Intense Laser Produced Plasma
85	Shri Asim Kumar Das	22.10.13	Design of an Undulator Based High Flux and High Resolution Beamline for Atomic & Molecular Physics Research
86	Shri Hari Sharan	25.10.13	Study and Development of Symbolic Simulation Techniques for Formal Verification of Hardware Design
87	Shri Raviteja Chilukuri	31.10.13	Seismic Isolation Strategies for Active Components Mounted on RCC Structures
88	Shri Saurabh Gupta	22.11.13	Static and Kinematic Analysis of a Suspended Servo-Manipulator
89	Ms. Surabhi Singhal	23.11.13	Study of Concurrency Control Mechanisms to Develop Collaborative Platform
90	Shri Ashish Kumar Shukla	25.11.13	Design Studies on Dome Shaped Roof Slab for Pool Type SFR
91	Shri Harsh Hemani	26.11.13	Comparative Study of Re-Meshing and Remapping



Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
92	Ms. Remya Haridasan	28.11.13	Study and Hardware Implementation of PSEC-KEM Protocol
93	Shri M. Anil Kumar Reddy (NFC, Hyderabad)	28.11.13	Study of Process Parameters of Uranyl Nitrate Raffinate (UNR) Treatment Process & Optimization
94	Subhojyoti Basu (NTC, Rawatbhata)	28.11.13	Study of Process Tomography in Imaging Multi-Phase Flow
95	Shri CH. Santosh Subudhi	11.12.13	Mathematical Modeling and Detection of Thermal Hydraulic Instabilities in AHWR
96	Shri Bommadeni Arun (BARC TS, Mumbai)	11.12.13	Prediction of Background in Low Energy Spectrum of Phoswich Detector
97	Shri Ashutosh Gupta	11.12.13	Algorithm Development for FPGA Applications in Mobile Gamma Spectrometry System
98	Shri Praveen Kumar	11.12.13	Shielding Analysis of the Transportation Cask for AHWR Fuel
99	Shri Nishith Ghosh	11.12.13	Study on Sound Attenuation Property of Polymeric Materials using Ear Simulator System and Pertinent Optimisation
100	Shri Avijit Das	11.12.13	Development of Three Dimensional Computer Code for Shielding Design of Nuclear Reactor
101	Shri Deepraj Paul	16.12.13	700 MWe PHWR-PHTS Mathematical Modelling and Control Study
102	Ms. Sushmita Bhartiya	16.12.13	Capacitive Deionization for Removal of Dissolved Heavy Metal Salts from Water
103	Shri T.S. Shri Krishnan	17.12.13	Development of Wi-Fi Based Gateway for Wireless Sensor Network
104	Shri Siddhartha Gantayet	01.01.14	Design of Robust Controller Using Periodic Output Feedback for Specific Power Range of Nuclear Reactor
105	Shri Balwant Singh	01.01.14	Study of Phase and Absorption Based Micro-Imaging Techniques
106	Ms. Pampa Modak	27.01.14	Study of Evolution of Aerosol Characteristics of Nanoparticles Generated Continuously in a Closed Chamber
107	Shri Nakul Raj Sethi	27.01.14	Modeling of Display Station Based Human Machine Interface for Nuclear Core Temperature Monitoring (CTM) System of Fast Breeder Reactor



Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
108	Shri Sujith K.R.	27.01.14	Design & Development of Diversified Real Time Computer for Fast Breeder Reactor Safety Systems
109	Atanu Mukherjee	28.01.14	Study of Alteration Associated with Microstructure of Mineralized and Barren Rock Along Gogi-Kurlagere Fault at Gogi Area, Yadgir District, Karnataka
110	Srinivasarao Bevara	28.01.14	Delineation of Geologic Structures using Magnetic Survey and Exloore the Structural Controls of Uranium Mineralization in Southwest Kerpura Area of Rajasthan
111	Vibhore Shrivastava	28.01.14	Characterization of Conducting Zones Favourable for Uranium Mineralization Using Induced Polarization (IP) & Transient Electromagnetic (TEM) Methods, Hirapur & Indora Areas, Bijawar Basin, Sagar District, Madhya Pradesh
112	Srinjoy Mukherjee)	07.02.14	Sedimentological and Geochemical Characterization of Lower Mahadek Sandstone in Wahkyn - Wahkut Area, West Khasi Hills District, Meghalaya
113	P. Shrajala	07.02.14	Delineation of Sulphide Rich Zones Using Induced Polarization/Resistivity Surveys and Exloore the Controlling Factors for Investigation of Uranium Mineralization along Parts of Albitite Line, Southwest Kerpura - Rajasthan
114	Arjun V.	07.02.14	Finite Element Model Based Optimization of Pulsed Eddy Current Probe for Sub-Surface NDE
115	Nipun	07.02.14	Despositional Environment, Paleocurrent and Provenance Studies of Badami Sediments vis-à-vis Basin Tectonics in and Around Deshnur Area, Belgaum Dist., Karnataka
116	Viney Kumar	07.02.14	Integrated Geophysical for Uranium Exploration in Parts of Surguja Shear Zone, Chattisgarh, India



Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
117	Ashim Jana	07.02.14	Establishing the Stratigraphy and Delineation of Major Structures within Siliciclastic Sequences Around the Southern Part of Deogarh and Mankarhachua Basins, Angul, Deogarh and Sambalpur Districts, Odisha for Identifying Favourable Zones of Uranium Mineralization
118	Sukanta Goswami	07.02.14	Role of Organic Matter in Uranium Metallogeny in Vempalle Formation
119	S. Srinivasa Rao	07.02.14	Modeling and Inversion of Gravity Data of Deshnur Area, Belgaum District, Karnataka
120	Boyapally Ravinder Goud	07.02.14	Structural and Geochemical Studies on Punagarh Basin with an Emphasis on the Alteration Patterns and Uranium Potential
121	Pratip Mitra	17.02.14	A feasibility Study on the Use of Silicon PIN Diodes for Environmental Gamma Monitoring
122	Gade Venkata Rajeev	14.03.14	Numerical Study of Passive Auto Catalytic Recombiner Using a Detailed Reaction Model
123	Amis Shankar	14.03.14	Two Phase Flow Modeling to Analyze the Operating Parameters of Thermo-Siphon Evaporators

Titles of M.Sc. (Engg.) Theses for which results were notified during April 1, 2013 to March 31, 2014

Sr.No.	Name of the Student	Date of Notification of degree	Thesis Title
1	Shailesh Kumar Mishra	20.05.13	Study of Turning Process and Effect of Vibration for SS 304 Components
2.	Shri Senthil K.	19.09.13	Study of Exploding Characteristics of EWA in Gaseous Environment



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Annex 6
Titles of D.M., M.Ch & M.D. Theses for which results were notified during April 1, 2013 to March 31, 2014



**Titles of D.M., M.Ch & M.D. Theses for which results were notified
during April 1, 2013 to March 31, 2014**

Sr.No.	Name of the Student	Date of Notification of degree	Degree	Thesis Title
1	Dr. Dongre Amol Shankar	11.07.13	DM-M.Ocly.	Clinical presentation and outcome of Hodgkin's lymphoma in children : A retrospective study.
2	Dr. Gautam Goyal	11.07.13	DM-M.Ocly.	An observational phase II study of efficacy of metronomic chemotherapy in patients with relapsed epithelial ovarian carcinoma with elucidation of its potential mechanisms of action by study of angiogenesis and apoptosis.
3	Dr. Partha Sarathi Roy	11.07.13	DM-M.Ocly.	Comparison of efficacy and safety of Rituximab (Mabthera TM) and its biosimilar (Reditux TM) in diffuse large B-cell lymphoma (DLBCL) patients treated with chemo-immunotherapy : a retrospective analysis.
4	Dr. (Ms.) Seema Ashish Gulia	11.07.13	DM-M.Ocly.	A prospective randomized, open-labelled parallel group trial of L-asparaginase vs. Prednisolone in a subset of newly diagnosed patients in acute lymphoblastic leukaemia presenting with hyperleukocytosis.
5	Dr. Sushant Mittal	11.07.13	DM-M.Ocly.	Utility of PET scan in early diagnosis of Bleomycin induced lung toxicity in Hodgkin's lymphoma patients.
6	Dr. Patil Vijay Maruti	11.07.13	DM-M.Ocly.	A prospective randomized phase II study comparing metronomic chemotherapy with chemotherapy (single agent cisplatin), in patients with metastatic, relapsed or inoperable squamous cell carcinoma of Head and Neck
7	Dr. Hasmukh Jain	11.07.13	DM-M.Ocly.	Treatment results in advanced stage Hodgkin's lymphoma : a retrospective study.
8	Dr. Prashanth Penumadu	11.07.13	MCh.- S.Ocly.	Retrospective audit of women with locally advanced breast cancer for extent of locoregional therapy for supraclavicular lymphnodes.
9	Dr. (Ms.) Nita Sukumar Nair	11.07.13	MCh.- S.Ocly.	A retrospective audit to evaluate the role of tumour quadrant in outcome, in women treated for early breast cancer at Tata Memorial Hospital.



10	Dr. Ritesh Satish Pruthy	11.07.13	MCh.- S.Ocly.	Retrospective audit of major salivary gland tumors presenting to TMH over a period of 10 years 2003-2012.
11	Dr. Sumeet Jain	11.07.13	MCh.- S.Ocly.	Retrospective audit of extremity malignant melanoma cases presenting to the Bone and Soft tissue Disease Management Group
12	Dr. Viraj Vijay Borgaonkar	11.07.13	MCh.- S.Ocly.	Correlation of pre-operative nutritional status with post-operative morbidity in head and neck cancer patients.
13	Dr. Wani Bhushan Navinchandra	11.07.13	MCh.- S.Ocly.	Quality of life analysis in patients who underwent maxillectomy.
14	Dr. Girish G.	11.07.13	MCh.- S.Ocly.	Enhanced recovery programme for patients undergoing surgery for Colorectal cancers.
15	Dr. (Ms.) Patkar Sharaddha Liladhar	11.07.13	MCh.- S.Ocly.	An observational study to analyse correlation between preoperative magnetic resonance imaging (MRI) findings and final histopathology report in cases of scar revisions performed for high grade soft tissue sarcomas.
16	Dr. Srikanth C.N.	11.07.13	MCh.- S.Ocly.	An observational study of microbes in oral cavity and post operative complications in patients suffering from malignant lesions of oral cavity.
17	Dr. K. Saravana Rajamanickam	11.07.13	MCh.- S.Ocly.	Quality of life analysis of throxine withdrawal versus triodothyronine supplementation in preparation for radiodine ablation in patients with differentiated thyroid cancers.
18	Dr. P. Dhanasekar	11.07.13	MCh.- S.Ocly.	Cut margin status and local recurrence in breast conservation therapy – A retrospective audit
19	Dr. Borkar Nikhilesh Ramkrishna	11.07.13	MCh.- S.Ocly.	Role of intraoperative cytology of fissuring dust from mandible specimen for bony margins of segmental and hemi mandibulectomy
20	Dr (Ms.) Deepti Mishra	11.07.13	MCh.- S.Ocly.	A retrospective case control study evaluating tamoxifen resistance in hormone receptor positive breast cancer – Role of Estrogen receptor Beta
21	Dr. (Ms.) Aekta Shah	11.07.13	MD-Pathlgy.	Retrospective audit of the results of ALK gene rearrangement by FISH in lung adenocarcinoma and correlation with histopathological subtype



22	Dr. (Ms.) Bhatkar Rohini Prakash	11.07.13	MD-Pathlgy.	Accuracy of frozen section evaluation of resection margins, tumour thickness and lymph node status in cases of squamous cell carcinoma of tongue
23	Dr. Motghare Priyal Krishna	11.07.13	MD-Pathlgy.	Sarcomatoid Neoplasms of the Breast Study of Morphological, Immunohistochemical features and Clinical outcome
24	(Ms.) Kante Katha Amol	11.07.13	MD-Pathlgy.	Nodal marginal zone lymphoma – From wastebasket to diagnostic sense
25	Dr (Ms.) Navale Pooja Prakash	11.07.13	MD-Pathlgy.	Can we apply WHO 2008 classification in acute leukemia cases in a tertiary care cancer hospital in India
26	Dr. Kulkarni Pranjali Prdeep	11.07.13	MD-Pathlgy.	Comparative study of oral cancers with and without oral submucous fibrosis with respect to the histomorphological variables and expression of biomarkers.
27	Dr. R. Vasanth Karthik	11.07.13	MD-Anaesly.	Effect of monitoring of cuff pressure on post-operative pharyngolaryngeal adverse effects after proseal laryngeal mask airway insertion
28	Dr. (Ms.) Kanineeka Das	11.07.13	MD-Anaesly.	To study the effectiveness of dexmedetomidine for sedation in elective awake fibre-optic intubation.
29	Dr. Ingole Advait Diwakar	11.07.13	MD-Anaesly.	A retrospective study of efficacy and side effects profile of epidural buprenorphine bolus analgesia Vs. epidural combined morphine and bupivacaine infusion analgesia after major abdominal surgery
30	Dr. Devawrat Ramdas Buche	11.07.13	MD-Anaesly.	Efficacy and side effects profile of continuous thoracic epidural analgesia vs. patient –controlled intravenous analgesia after major surgery.
31	Dr. Alok Ranjan Sahoo	11.07.13	MD-Anaesly.	A prospective randomized trial to compare success of insertion of the Proseal LMA using classic digital technique versus gum-elastic bougie-aided technique.
32	Dr. (Ms.) Deepshikha Palit	11.07.13	MD-Anaesly.	A prospective, randomized controlled comparative study between triamcinolon acetonide paste and lignocaine jelly applied over tracheal tube to reduce the incidence of post-operative pharyngolaryngeal complications.



33	Dr. (Ms.) Afroz Shahana Mehboob Khan	11.07.13	MD-Anaesly.	A prospective observational study – epidural catheter insertion site and adequacy of post-operative pain relief in children undergoing thoracic and upper abdominal surgeries.
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42	Dr. (Ms.) Deshpande Sneha Satish	11.07.13	MD-Rad.Diagn	Computed tomography pulmonary angiography : Impact of patient's body mass index on contrast enhancement
43	Dr. Bhagwat Mahesh Rajaram	11.07.13	MD-Rad.Diagn	Prospective study – comparative study of plain and contrast CT scan of thorax, to compare efficacy of plain scan with contrast enhanced scan to detect pulmonary parenchymal metastases in patients of bone and soft tissue sarcomas.



44	Dr. (Ms.) Ashwathy Susan Mathew	11.07.13	MD-Rad.Thy.	A Prospective study of telephonic contact and subsequent physical follow up of radiocally treated lung cancer patients.
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52	Shri Amit Sharma	09.01.14	MD-Rad.Thy.	A Dosimetric comparison of Boost with HDR interstitial Brachytherapy and with external beam techniques with electron, 3 DCRT and Tomotherapy
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MACE telescope proof-assembly designed and developed by BARC & installed at Hyderabad.

DIRECTOR

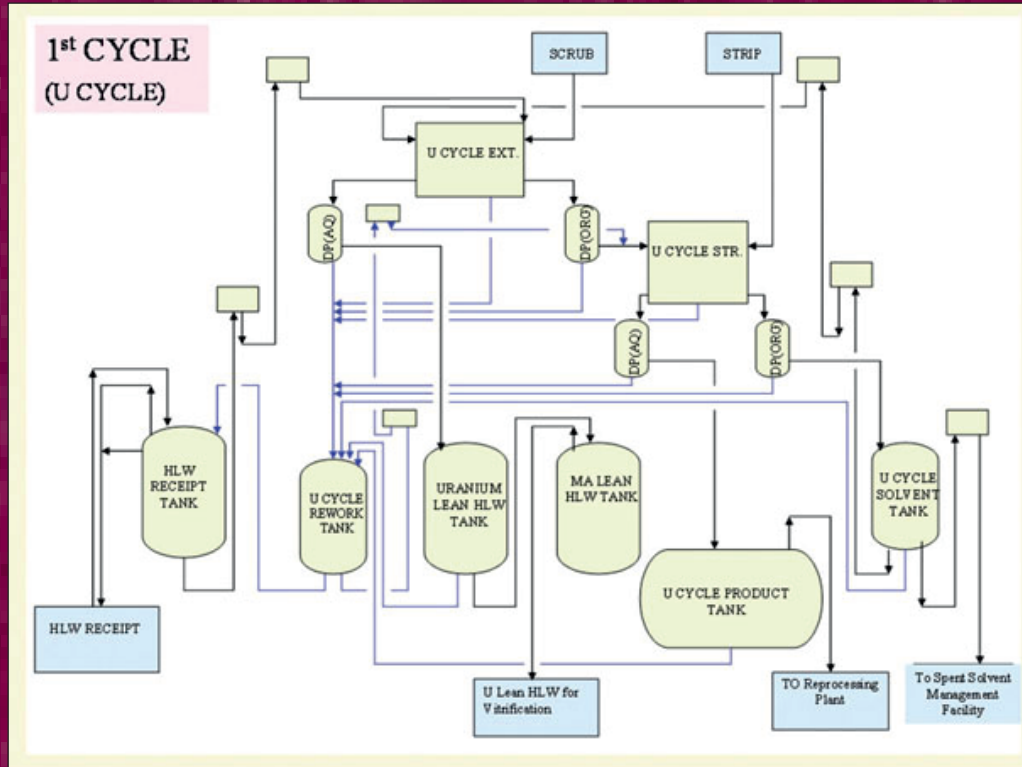
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