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Founder and Architect of the Indian Atomic Energy Programme

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From the Director's Desk.

Human Resources Development Initiatives at Indira Gandhi Centre for Atomic Research



"Our minds are finite, and yet even in these circumstances of finitude, we are surrounded by possibilities that are infinite, and the purpose of life is to grasp as much as we can out of that infinitude"

- Anonymous

Indira Gandhi Centre for Atomic Research has the mission to develop robust, safe and economical fast spectrum

reactors with closed fuel cycle, contributing to the energy security for India in the 21st century. Fast spectrum with closed fuel cycle energy system is preferred by advanced countries for energy security in a sustainable manner with limited burden on the environment. Human resources, capable of pursuing mission in a seamless manner from science to technology deployment, are a key to success for such a challenge and opportunity. Development of human resources requires mechanisms, teachers par excellence, resources and passion for nurturing and providing capacity and capability to young generation. True satisfaction can accrue to those who can achieve human resources development in a holistic manner. Holistic perception of human resources development at Kalpakkam includes environment of learning with fun, but with intensity, art of growing up with confidence and passion to serve the country, excellent townships, schools, hospitals, green and clean environment and care for the neighbourhood villages.

Dr. Homi Jehangir Bhabha, whose centenary we are celebrating during October 2008 -2009 was a true champion of holistic human resources development with sensitivity to the society. I have thought of writing this article in the centenary year to offer my salutations. The article outlines our initiatives, in the recent years, for enhancing the human resources development at the Centre.

Initiating the Training School programme at our Centre, identifying research problems in interface areas for achieving breakthroughs to be taken up by the young research scholars, attracting young persons and empowering them has been the 'mantra' adopted at the Centre. We have also tried to utilize the vast potential available in the academic institutes and R&D organizations. To bring the equity to the neighbouring villages, we have initiated programs to enhance the learning opportunities and provide training opportunities in vocational trades, improving hygiene and health care. I would be highlighting some of the Human Resources Development measures undertaken by our Centre and also touch upon multilevel mentoring process, which has been built in our system.

Training School

To nurture young talents in order to meet the urgent and growing need of

"The building itself is only a shell to make possible the work that is done inside it. It is by the quality and volume of its scientific work that an institute like this must be judged, by the extent to which it has helped to explore and push back the frontiers of knowledge, to open up new fields of knowledge, to provide the country with men highly trained in the newest fields of scientific endeavour and able to make their own contribution to the increase of scientific knowledge and by its general impact on the scientific life of the country as a whole"

-Homi Jehangir Bhabha

scientific human resources with the right training, the Training School for fresh engineers and science post-graduates in physics, chemistry and materials science Orientation course for young engineers and scientists(OCES) was started in September, 2006 at Kalpakkam. The trainees, on successful completion of training, have been placed mostly in IGCAR and also in various other Units of DAE. Initially, the training programme was conducted in three disciplines (viz.) mechanical, electronics & instrumentation and chemical engineering with orientation towards Fast Reactor and associated Fuel Cycle Technologies. Realising the need to address R&D challenges in chemistry of fuel cycle and reactor physics for success in Fast Breeder Reactor and closing the fuel cycle technologies, training programme in Nuclear Fuel Cycle Chemistry and Nuclear Reactor Physics have been commenced in the year 2007. Training in these courses will generate quality manpower for taking up the challenging issues relating to reactor physics, safety, processing of nuclear materials including reprocessing and waste management. Taking into consideration, the decrease in the number of metallurgy graduates joining the Training School programme and to cater to the sustained demand for materials science specialists, the training programme

in materials science stream is being conducted from 2008. The best of the experts from our Department were selected for teaching, majority of them from IGCAR. We have also utilised the expertise available in reputed academic institutions like Indian Institute of Technology, Madras and Anna University, Chennai. Special lectures and visits to the laboratories have been a part of the curriculum for the Trainee Scientific Officers. Evening interaction sessions at the Training School hostel with eminent personalities from India and abroad are organised which form a part of continuous mentoring exercise. The training programme is conducted with holistic perspective to nurture and shape the young talent towards taking up the challenges of the Centre and the Department.

The salient features of the training school programme is to impart fundamentals and experience by practicing professionals thus ensuring that implicit and tacit knowledge is shared and cultivated. Continuity of intake and training sets a "Chain Reaction" ensuring that trained manpower is available at all times. Security of a job to those selected for training ensures their commitment and new training programmes introduced ensure supply of expert manpower according to changing nature of the requirements of the Department. About one hundred and eight students have graduated from BARC Training School at Kalpakkam since its inception and have been placed in various Units of the Department like BARC, NPCIL, NFC, AERB and BHAVINI apart from IGCAR.

Research Scholars

We also realised that in order to leapfrog to the future, challenges in R&D related to FBRs operating on advanced fuel with inherent safety and economy have



Glimpses of interaction sessions of students with distinguished visitors to the centre

CHALLENGES IN SCIENCE AND TECHNOLOGY

FBTR life extension for next 20 years Realising Fast Reactor Fuel Cycle Facility

Design and development for 500 MWe FBRs with improved economy and enhanced safety

High performance fuel cycle technologies

Significant progress towards realisation of metal fuelled reactor and associated fuel cycle technologies

Science

- Materials and their performance under high temperature, sodium, irradiation environments over the long reactor life
- Development of non-metallic materials operating at high temperatures and radiation environments (special high density concrete, elastomers, ceramics, cables, etc.)
- Sodium chemistry, aerosol behaviour, sodium fire and sodium water reactions
- Special sensors for sodium applications (detection of water leaks in steam generator, sodium leaks, purity measurements, level detectors)
- Thermal hydraulics and Structural mechanics (turbulences, instabilities, gas entrainments, thermal striping, stratifications, ratcheting, etc.)

Engineering

- Design of components at high temperature and long life
- Design of mechanisms operating in sodium and argon cover gas space
- Design to accommo-date sodium leak and sodium water reactions
- Seismic design of interconnected buildings, components and thin shells with fluid-structure interaction
- In-service inspection and repair of reactor internals, High temperature fission chamber

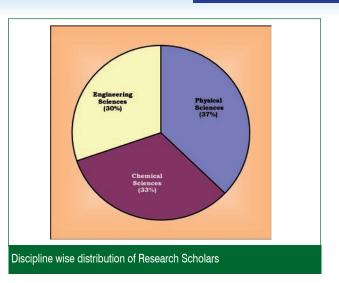
Technology

- Manufacture of large dimensioned welded thin shell structures made of austenitic stainless steel petals with close tolerances(~thickness) (e.g.) Main and safety vessels, inner vessel, thermal baffles, etc.
- Machining of large dimensioned and tall slender components with stringent tolerances (grid plate, absorber rod drive and component handling systems)
- Fabrication of large size box structures with controlled distortions
- Hard facing technology
- Development of Inflatable seals and large size bearings

"There is no genuine knowledge in the universe that is not potentially useful for man, not merely in the sense that action may one day be taken on it but also in the fact that every new knowledge necessary affects the way in which we hold the rest of the stock"

-Homi Jehangir Bhabha

to be addressed. We believe that the approach to solving most of the challenges is by practicing science based technologies which is based on solid foundation of physics, chemistry and engineering. This approach would enable us to achieve breakthroughs, and also



provide for an adequate reservoir of knowledge base in frontline technologies. In order to realize our goals, we have inducted young research scholars into our vibrant R&D programs. The strength of the research scholars in the Centre has been steadily increasing from fifteen thirty five years ago to a present strength of over hundred. The sanctioned strength is two hundred. We have identified the research areas which have a direct bearing on the mission related activities of the Centre, Research scholars will be pursuing research in interdisciplinary fields that links basic sciences with engineering, such as physics and reactor engineering, chemistry and chemical engineering etc. This approach promotes the involvement of basic sciences in challenging mission programmes of the Centre and also provides opportunities for original research and possibilities for breakthroughs. While allotting the students, we are ensuring that the guides have the credibility of a mentor, ability and his/her own quality of research. The research scholars pursuing their doctoral programs are evenly distributed in physical, chemical and engineering sciences.

Some of the research areas being pursued by research scholars

Engineering Sciences

- · Gas entrainment in liquids
- Improved safety with liquid metal
- Material modeling with micromechanics based approach
- Complex thermal hydraulics and two phase flow
- Computational Fluid Dynamics and power plant dynamics
- Seismic integrity assessment
- Advanced civil design with interconnected structures
- Prediction of ageing and damage mechanisms for long and reliable plant life with Non Destructive Evaluation techniques

Fuel Cycle

- Bulk separation processes at extremely low concentrations
- Single molecule spectroscopy
- Microstructure tailoring to achieve near zero corrosion rate
- · Design with enhanced conceptualisation and modelling
- · Modelling to enable long life systems

Mentoring

"I've learned that people will forget what you said, people will forget what you did, but people will never forget how you made them feel"

-Maya Angelou

Mentoring has the highest priority in the activities of the Centre. I believe that mentoring is a worthy proposition to achieve success in realising mission and vision of high technology domains of national relevance and importance. Our multi level mentoring strategy lies in the Director empowering the Group Directors for effective management and implementation of programmes. The Group Directors in turn advise and coordinate the research activities with Division Heads, who ensure effective control and monitor the academic and financial milestones of individual sections in their Divisions. The Heads of Sections nurture the talent and skills of engineers/scientists working with them. The scientists and engineers ensure proper guidance to the technical staff for execution of the work. There is a direct and free access to individuals at all hierarchical levels of management with a "Meet me" approach without barriers. Periodic mentoring exercises and continuous mentoring to younger colleagues outside the hierarchical system, has paid rich rewards, to reduce bureaucracy, to unshackle the inhibitions and inspire the young persons to be bold in their initiatives and approach to realise their limits of success.

We have organised periodic "orientation programmes" for young and directly selected scientists and engineers thus enabling them to get an exposure to various activities of the Centre by way of lectures by senior colleagues and visits to various facilities. Lectures are also arranged to teach the basics of core subjects like reactor physics, health physics, fuel cycle chemistry, reactor engineering etc. which are necessary to all the officers irrespective of their assignments. These orientation programmes give the fillip to the formal training, which they lack, when compared to an officer graduating from training school.

Empowering the employees

"An empowered organization is one in which individuals have the knowledge, skill, desire, and opportunity to personally succeed in a way that leads to collective organizational success"

-Stephen Covey

The Homi Bhabha National Institute set up in the year 2005, caters to providing avenues to employees to improve upon their qualifications. This serves a dual purpose of achieving higher satisfaction levels amongst the staff members and also in updating their knowledge base. Employees pursue Masters and Ph.D. Programmes under the aegis of HBNI. There are more than 100 employees pursuing M.Sc.(Engg.) and Ph.D.s presently and 78 officers graduated from

the recent batches of the training school are pursuing M.Tech. programmes. Specialised and advanced courses have been formulated to cater to the needs of employees for enhancing the knowledge base. I have participated, at all stages, right from the inception to the current stage, as a member of governing council and advisory board. I and my colleagues are committed to harness the full spectrum of advantages brought to the Centre under the auspices of HBNI.

Award and Reward Schemes

"In the arena of human life the honors and rewards fall to those who show their good qualities in action"

-Aristotle

DAE has instituted annual awards for excellence in Science, Engineering and Technology in order to identify best performers in the area of Research, Technology Development and Engineering in the constituent units. The Young Scientist, Young Technologist, Homi Bhabha Engineer, Young Science and Technology Award and Scientific and Technical Excellence Award fall under this category. Group Achievement awards for recognition of major achievements have also been instituted. Life time Achievement Award is awarded to one who has made significant impact on the DAE's programme. They are the icons for young scientists and engineers to emulate. The award schemes are targeted to motivate the employees. I am happy to note that a good number of employees from our Centre are being bestowed upon by these awards.

Collaborations

"The relative roles of indigenous science and technology and foreign collaboration can be highlighted through an analogy. Indigenous science and technology plays the part of an engine in an aircraft, while foreign collaboration can play the part of a booster. A booster in the form of foreign collaboration can give a plane an assisted takeoff, but it will be incapable of independent flight unless it is powered by engines of its own"

- Homi Jehangir Bhabha

In order to meet the challenging tasks in our indigenous mission programme, we have worked, over the decades, to network a vibrant academiaresearch institute-industry interaction, towards finding solutions for FBR and associated closed fuel cycle technologies. The various modes of interaction with academic and research institutes include participation of students to pursue postgraduate research at our Centre, sponsored research projects under the aegis of Board of Research in Nuclear Sciences (BRNS), collaborative projects and by organizing vocational training courses and workshops. DAE Young Scientist Research Award, Dr.K.S.Krishnan Research Associateship, DAE-BRNS Senior Scientist Scheme and DAE Graduate fellowship are some of the avenues to attract talent to participate in our programmes.

Apart from the contributions from eminent faculty members, the inputs provided by the dynamic and enthusiastic students have been commendable. Inter-University consortium-DAE Facilities Nodal Centre has been set up to serve as an interface between DAE organizations and the academic institutions. IGCAR has been organizing annual "summer training programmes in basic sciences" to create a fraternity and inspire young students from academic institutions to take challenging careers in Science. It is heartening to note that several of them have written back to us to emphasize the usefulness of the training and guidance at IGCAR in shaping their research and careers.

"I and my family sincerely thank you for the special interest you showed, which paved the way and brought me here. If I could do something, get a Ph.D., all because of the support and encouragement I had from various sources with IGCAR topping the list"

- Dr. Arul Murugan, Ferrotec, Japan

"The two summer internships at IGCAR acted as a real guiding light in enabling me to understand and work in my field of interest. The internship after my first year at IGCAR equipped me to work on projects along with seniors which won national level competitions"

- Shri G.Gokulavasan, BITS Pilani

"I feel IGCAR has well established the principle of 'Yatha Raja Thatha Praja'. IGCAR was a place for me where I got something more than what I wanted. I was literally shocked looking at the huge library getting everything you asked for. I still wonder about the good treatment that IGCAR showed to an undergraduate like me. Talents are always respected and encouraged at IGCAR. I am really thankful to Dr. Baldev Raj sir for giving me this golden opportunity and IGCAR for giving me so many things"

- Shri Sagar Prabhuder, NITK, Surathkal

R&D through collaborations have helped in generating critical inputs in shorter than expected time, development of several centres of excellence, technology development exercises have paved the way for incorporating up-to-date manufacturing and inspection technologies for manufacture of large and precision engineered components. International collaborations promote inter-laboratory cooperation and hybridization of ideas. These are beneficial to the Centre as well as the participating institutions.

Our scientists and engineers have had the opportunities of working in many of the international laboratories, and the researchers from abroad have come to our Centre for working in areas of common interest. We have collaborative projects with ninety four research institutions out of which eighteen are international with institutes like IIT-Madras, IISc, Bengaluru, NCL, Pune, UICT, Mumbai, we have also initiated mega collaborative efforts, by way of establishing research facilities.

A flavour of collaborations which have yielded excellent results
* Design and establishment of Wireless Sensor Networks for Nuclear Applications- <i>Collaboration with Anna University</i>
* Fabrication of yttria doped thoria (YDT) thimbles and glass soldering them to Fermi alloy component towards development of oxygen sensor for use in sodium coolant of Fast Breeder Reactor- <i>Collaboration with CGCRI</i>
* Development of a CFD Model for Blockage of Coolant flow path in Fast Breeder Reactor Fuel Sub-Assembly- <i>Collaboration with IIT Madras</i>
* Thermal Stratification in molten sodium pool- Collaboration with UICT, Mumbai
* Development of ferritic ODS clad tube- Collaboration with ARCI and NFC
* Biodiversity studies in the coastal waters of Kalpakkam- Collaboration with Loyola college, Chennai

Recently, we have also initiated an exercise to identify the 'gap areas', in each discipline, where research can be pursued by the fresh Ph.D. student, to enrich R&D for the mission programmes of the Centre and the Department.

Neighbourhood Development Programmes

"The unselfish effort to bring cheer to others will be the beginning of a happier life for ourselves"

- Helen Keller

In order to instil confidence and to develop a general feeling of well being amongst the people living in the surrounding villages, we are earmarking funds towards providing avenues for learning and acquiring vocational skills, thereby enhancing the knowledge base, providing health care and several other welfare programmes including hygiene, clean water, radio station at Kalpakkam, empowering women etc. An integrated approach by all the units of DAE located at Kalpakkam towards enriching the quality of life in the neighbourhood villages is an important part of our mission.

Imparting Vocational Training and Education to Rural Youth

"We want that education by which character is formed, strength of mind is increased, the intellect is expanded, and by which one can stand on one's own feet"

-Swami Vivekananda

Vocational Training Programme is being conducted to train the unemployed youth for the development of their vocational skills in various disciplines such as plumbing, carpentry, electrical works etc. This training helps the village youth in self-employment. This programme is in line with ITI training for better employment prospects of youth of neighbouring villages. A year-long vocational diploma enabling

young boys and girls to work as electricians, lab technicians, hospital workers, plumbers and welders, is jointly imparted by the Sathyabama Deemed University and the Kalpakkam Management Committee at Kalpakkam.

The Indian Society for Non-destructive Testing (Kalpakkam Chapter) is conducting Level I courses to empower the village youth in Non-destructive testing methodology which can fetch excellent job opportunities upon completion of the course. About one hundred students from neighbourhood have been trained in NDE courses. Students coming from seventeen villages including Sadras, Vasuvasamudram, Pudupattiman, Vayalur, Venpurusham, Suradimangalam, Kadambadi, Neykuppi and Natham are already assured of their job. The trained manpower from this programme can also supplement the semi-skilled/skilled manpower needs of the DAE installations. It really inspires to realize that several of them have good careers with suitable salaries. Distance education programmes through Indira Gandhi National Open University and Sankara College have also helped several youth from lower strata of the society, to obtain their graduation and moreover gain confidence to realise their dreams in life.

Infrastructure improvement in Educational Institutions

"Education is the great engine of personal development. It is through education that the daughter of a peasant can become a doctor, that a son of a mineworker can become the head of the mine, that a child of farm workers can become the president of a nation"

-Nelson Mandela

Holistic approach to education which puts emphasis on learning, building skill sets, appreciation of ethics and sensitivity to all stakeholders in society and wealth generation, is key to India progressing in to a developed nation. Taking into account the population of the neighbouring villages and poor literacy levels, we have embarked upon improvement of infrastructure and facilities for the schools like provision of laboratory equipments, computers, libraries, teaching aids and reference materials etc. These programmes are aimed at improving the incumbent level in the school are sure to increase the literacy in the villages. We have also formulated schemes to impart education and provide support equipments to take care of the physically and/or mentally challenged children.

In summary

Science Management is simple; as simple as science itself. To pursue science management, you need simplicity, honesty and self confidence. Science management is all about facing realities, encouraging "Create an environment of Meritocracy: Spot and track nascent talent and create leaders with a rich mix of skills – who have exposure to different functions in the organization. Time and again, the supremacy of the human skill and spirit cannot be over-emphasized. The success or failure of an organization depends on human beings, their talents, their initiatives, their ability to lead and co-ordinate with others and importantly, to work as a competitive team. It also depends on the ability of the organization to motivate them to greater heights and to provide necessary challenges..."

- Aditya V. Birla

individual style and mavericks as long as they are committed to pursuits. One must avoid followers who are not committed to science pursuits and their excellence. It is important to encourage changing paradigms and new worthy issues and problems. Science management is using the brains of your colleagues to discover the best ideas by interactions and capacity to implement these ideas at fast pace. Science management requires innovations in cutting down bureaucratic layers towards enhancing effectiveness of individuals and teams. Science management is an art of creating bliss and fulfillment for you and your team.

"It is my belief that capacity and capability, confidence with conviction, faith in teams, selfless and egoless, work passion with sensitivity to colleagues, peers and deprived citizens, commitment to the vision and transparent communication of articulated vision to involve many, are the hallmarks of science & technology leader who aspires to achieve mega success of value to society"

-Baldev Raj

Our strategy of Human Resources Management is for implementing clear and definite mission with vision. Effective and sensitive management style with ethics, decentralization for proper and optimal utilization of financial and human resources, empowerment of designated persons for expeditious decision making, periodic monitoring of technical and financial milestones, encouraging excellence in all domains of science, engineering, technology, management and promoting cross-fertilization of good ideas across the groups are the enabling tools for us to realise successes and world leadership in our chosen domain of pursuits, namely, Robust, safe and economical Fast Spectrum Reactor with Associated Closed Fuel Cycle for the energy security of the nation.

Bulder Rj

(Baldev Raj) Director, IGCAR

Challenges in the Design of Mechanisms Working in Sodium for FBR

echanism is a term applicable to any device that IVI is used to effect motion transfer and to convert one type of motion to another, like conversion of rotary to linear or reciprocating to oscillatory etc. The absorber rod drive mechanisms, fuel handling machines, sodium pumps, failed fuel location module, neutron detector handling mechanisms, under sodium ultrasonic scanner are some of the mechanisms working in sodium in fast reactors. What makes the design of these mechanisms a challenge? Mechanisms are generally designed very rigid to ensure faithful transmission of motion and functional requirements rather than stresses developed govern the design. Hence formulating code rules for design, based on stress levels is not useful This article aims at bringing out the challenges in the design of mechanisms working in sodium for fast breeder reactors.

The foremost challenge is to design the mechanisms very compact in order to achieve overall economy. The use of compact core in fast reactors results in restricted space for the absorber rod drive mechanisms located directly above the core. The other mechanisms mentioned earlier are located in the top shield and are also designed very compact with minimum size and weight. The compactness is required in order to achieve minimum main vessel diameter, which is considered as a yardstick in FBRs for an economical design.

The other major challenge comes from the sodium environment in which the mechanisms are operating. The sodium coolant, though very good for heat transfer is not good for the mechanism elements. Sodium is opaque, which makes all the mechanism operations a blind one. This calls for remote operation of the mechanisms using feedbacks obtained from various instrumentation provided to sense the desired motion. Usually, these instrumentations are redundant and diverse. Sodium also generates large quantities of aerosols in the cover gas space above the sodium level. These aerosols are transported to the annular gaps in the mechanisms and have a tendency to deposit and solidify obstructing the motion. This calls for temperatures to be maintained above 373 K in the top shield, higher than the melting point of sodium.

The coefficient of friction in sodium is higher (generally 2 to 2.5 times) leading to increased drive power. The higher operating temperatures in FBR also require appropriate material selection suitable for the temperature range and compatible with sodium. Austenitic stainless steel 316 / 316LN with good high temperature strength and ductility is used for parts immersed in sodium. Where high strength and hardness is required, precipitation hardened steel ASTM A 453 Gr 660 material is used due to its very good mechanical properties and excellent compatibility with sodium. Even though most of the drive elements like gears, shafts, couplings etc. are located above top shield in the low temperature regions, guiding surfaces in contact with sodium as mentioned earlier are inevitable which give rise to the possibility of galling or self welding. Hardfacing and use of materials with high strength & hardness like the precipitation hardened ASTM A 453 Gr 660 are the solutions implemented to overcome the above problem. Here again, because of the radioactive environment, the choice of hard facing alloy is limited. colmonoy, which is a nickel base alloy is preferred over stellite, a cobalt based alloy to reduce radiation exposure of maintenance personnel due to induced radioactivity. The colmonoy deposition over austentic stainless steel is a real challenge and has been mastered after many development trials. Since colmonoy deposition is similar to a weld deposit, it induces distortion, requires heat treatment after rough machining & deposition and finish grinding of hard deposited surface to get the final dimensions. In some cases, the geometry of the mechanism element (like the Inclined Fuel Transfer Machine rails shown in Figure 1) is guite slender inducing significant distortion during colmonoy deposition which makes each and every component with deposition a unique case requiring trials and procedure qualification to establish the process. Colmonoy deposition on ferritic steel is even more challenging and achieving a defect free deposition free of cracks with minimum



Figure 1: Inclined Fuel Transfer MachineTilting Rails

repairs is a tough task. Figure 2 shows the dashpot piston of Diverse Safety Rod Drive Mechanism (DSRDM) during hardfacing trials and qualification with 9Cr-1Mo as the base material.

The opacity of sodium also makes in-service inspection, maintenance, and intervention for any in-situ rectification for malfunctions observed during service very cumbersome. The lack of feasibility of visual observation calls for designs with very high reliability to ensure minimum intervention during service. The reliability needs to be established based on fault tree analysis and detailed reliability studies. Also innovative techniques need to be developed as and when the need arises and depending on the magnitude of the problem observed. The variety of tools and techniques developed and employed during the guide tube incident in FBTR is a shining example. Use of simple and reliable designs, provision of reliable instrumentation, step by step sequence of operation with provision of interlocks based on feedbacks from the instrumentation, use of skilled manpower for operation, imparting adequate training for the operators, use of training simulators to periodically qualify operators are some of the measures adopted to avoid serious incidents.

In the design of mechanisms, specification of dimensional tolerances and tolerancing studies including cumulative buildup of tolerances and its effect on required functional requirements needs to be studied in detail. The phenomenon of radiation induced bowing is another major concern area, specific to fast reactors, which results in significant deviation (~20 mm) in the position of the top of the heads of subassemblies from their theoretical positions. Adequate flexibility must be provided in the portion of mechanisms interfacing with the subassembly. This is conflicting with the general



design approach of designs with rigidity and calls for optimization for certain elements where flexibility is also essential. This is especially important for both the shut down system mechanisms and the fuel handling machines. This also calls for kinematic analysis taking flexibility of the elements also into account. Figure 3 is a typical illustration of the situation where the electromagnet of DSRDM is being lowered into diverse safety rod (DSR) subassembly with 30 mm misalignment between their axes. Similarly, the dilation or radiation induced change in cross section of the subassemblies coupled with bowing gives rise to mechanical forces between adjacent subassemblies which results in additional forces to be applied during extraction/insertion of the subassemblies into the core. For example, the transfer arm, the in-vessel handling machine is designed with an extraction force capability of 15kN and an insertion capability of 10kN. Development of core structural materials resistant to swelling which would lead to reduction/



Figure 3: DSRDM & DSR with 30 mm Misalignment

elimination of bowing/dilation would help to offset this problem.

The high chemical activity of sodium with both air and water leads to difficulty in direct intervention and requires sodium cleaning before any maintenance activity is carried out. Designing with adequate features favoring sodium draining with minimum sodium retention is an essential requirement. The sodium sticking to the elements of mechanism is converted to stable inactive forms before they are washed with water. After sufficient residence in the reactor, the mechanisms also accumulate deposits of corrosion products which are radioactive in addition to induced radioactivity of the material of construction especially for the portions closer to the core. This calls for procedures for chemical decontamination of the components prior to maintenance. Figure 4 shows a typical photograph of DSRDM after sodium cleaning.

Provision of clearances/annular gaps is inevitable in order to effect motion transmission. However, these gaps/clearances lead to radiation streaming. Provision of bulk and complementary shielding based on detailed shielding studies is made to ensure adequate radiation protection to operating / maintenance personnel. The annular gaps also lead to natural convection of the argon cover gas coupled with the transport of sodium vapour leading to vapor deposition in the cooler zones of mechanisms. Detailed thermal hydraulic analysis is carried out to ensure that temperatures are maintained above

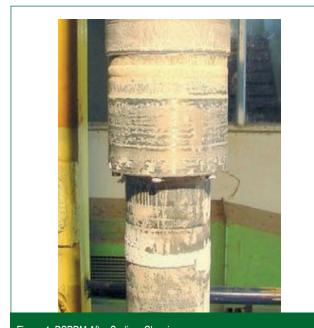


Figure 4: DSRDM After Sodium Cleaning

373 K to avoid sodium deposition. Similarly, detailed seismic analysis and flow induced vibration studies are made to ensure functional limits are met for satisfactory performance of the mechanism.

Provision of oil lubrication of mechanism parts is also a critical issue due to possibility of oil ingress with resultant positive reactivity addition due to entry of hydrogenous material into the core. For the primary sodium pumps, oil is used as lubricant above roof slab with adequate provisions to detect and monitor the level of oil. For the sealing below sodium free level, a hydrostatic bearing wherein sodium is pressurized and sent to a small annulus between the shaft and the mating part to maintain a film of lubricant is used. However, this calls for stringent requirements during manufacture of the pump components to maintain the radial gap and maintenance of verticality of the pump during operation.

Having discussed the challenges so far and designing mechanisms to overcome these challenges, can we say with confidence that the mechanisms will work satisfactorily? Since the mechanisms are an assembly of many parts with relative movements and motions, a number of factors decide their successful performance including the specific influences of sodium. Hence, the approach followed is to manufacture full scale prototypes and to qualify them by performance testing mostly both in air and in sodium.

Design of mechanisms working in sodium for FBR is thus a multidisciplinary effort which includes machine design, structural analysis, thermal hydraulic analysis, shielding analysis, material selection, hardfacing, electrical and instrumentation, technology development, manufacture and testing. It provides scope for multi disciplinary design analysis and R&D efforts including collaborative efforts with research/academic institutions. It is mostly the functional requirements, which govern the design precluding the development of standardised design codes. Successful performance of the mechanisms depends on simplicity and robustness of the design and validation of the design by prototype scale testing under conditions similar to the actual service.

(Reported by R. Vijayashree and colleagues, Components Handling & Mechanism Division, NEG/REG)

Atmospheric Flow Field Modeling at Kalpakkam: Initiation of a Multi-institutional Collaboration

Ctudy of dispersion of radioactive releases is of Vital importance for safe design and operation of nuclear plants for sustained power production and for environmental safety. The key issue of environmental pollution from nuclear facilities is the radiological impact due to the releases occurring from normal operation and in unlikely events of accidental conditions. Modelling the spread of radioactivity through air, water and soil media is an important step in assessing the radiological impact in the environment. The transport and dispersion of effluents in the atmospheric medium are determined by the flow field and its degree of turbulence at any given location. Flow field of the atmosphere unlike in the case of soil and aquatic media, is highly turbulent and is characterized by the regional weather pattern and the topography of a given site. Atmospheric circulations of various spatial and temporal scales act on the plume and determine its dispersion near to the source, locally and far-away. Atmospheric flow field though largely driven by regional circulations, within the lower few kilometers above the ground called the atmospheric boundary layer, the terrain and surface heterogeneities induce local scale circulations which will have significant impact on the plume trajectory and pollutant distribution. For instance complex topography, sea-land interface, heterogeneous land cover etc., at coastal and hilly sites lead to the development of terrain induced meteorological flows. The air concentration and deposition pattern of the radioactive effluents would be complex under these localized flow conditions and need to be represented carefully in dispersion calculations.

The meteorological issues in the dispersion of atmospheric releases is the availability of high resolution wind data to capture the variations in the flow and turbulence that generate the spatial and temporal variable concentration / dose pattern from the source. Essentially it is important to simulate the atmospheric flow at three spatial scales i.e., micro (~2 km), local scale (up to 10 km) and mesoscale regimes (~100 km). In the micro-scale, bluff body objects like buildings of various facilities

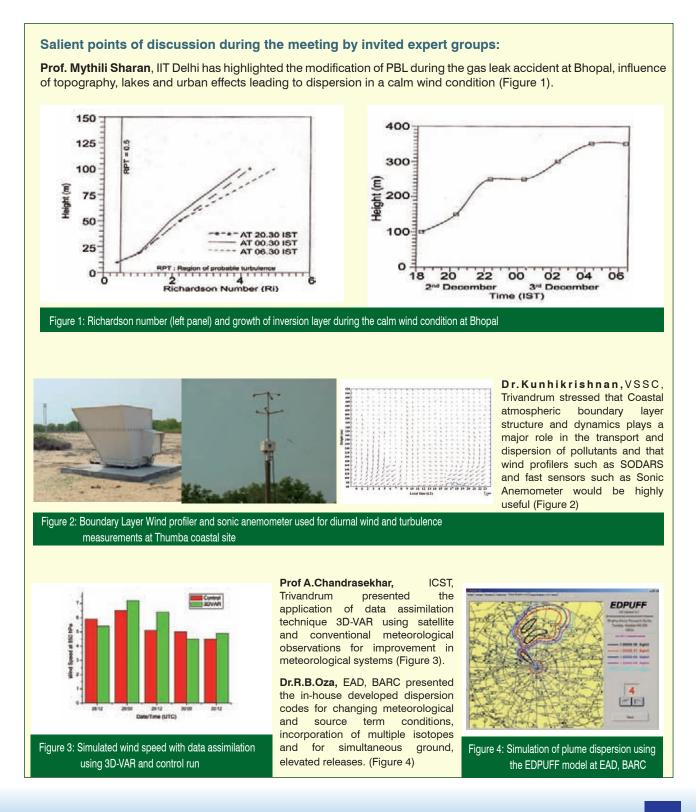
and plant canopies modify the flow field leading to wake generation and variable velocity along the streamline. In the medium scale the variability in the surface roughness due to the array of topographic objects within a small fetch of ~10 km influence the flow. In the mesoscale topographic flows such as the land-sea breeze at the coastal site, mountain-valley circulation at hilly stations and urban heat island effects in cities alter the diurnal flow and mixing depth in the atmosphere. At a coastal site as in Kalpakkam all the above flow features become important in the transport and diffusion processes and need to be realistically simulated for accurate assessment of atmospheric dispersion at specific distance ranges. Several techniques have been in vogue to simulate the atmospheric flows using various approaches. Diagnostic, prognostic and Computational Fluid Dynamics models based on numerical methods are widely used to simulate the three dimensional flow and turbulent quantities. Field experimental observations provide the basis to validate these models and to develop confidence limits.

A Round Robin Exercise has been initiated by Radiological Safety Division (RSD), IGCAR on accurate wind flow simulation for Kalpakkam coastal site for the study of atmospheric dispersion involving premier research institutions like IITs, universities and other national laboratories. The goal of the exercise is to devise state-of-the-art validated models suitable to specific spatial ranges for their implementation for atmospheric flow field simulation at the Kalpakkam site. Thus, it is needed to inter-compare various approaches/methodologies/models and evaluate the performance of the model with respect to observed meteorological parameters. Under this exercise, different research groups perform wind field modeling using the same set of bench mark data, intercompare and validate the results.

A technical discussion meeting was convened to formulate the Round Robin Exercise during August 13-14, 2009 at our Centre. About twelve research groups involved in theoretical and experimental studies from premier institutions in India like IIT, ISRO, IITM (Pune), Andhra University, Jadavpur University apart from the scientists from the units of DAE participated in the meeting. The proceedings started off with an inaugural address by Dr. P. Chellapandi, Director, Safety Group followed by presidential address by Shri H.S.Kushwaha, Director. HS&EG, BARC and a Keynote address by Prof. Mythili Sharan, of Centre for Atmospheric Science, IIT- Delhi. Dr. A. Natarajan, and Shri A.R. Sundararajan, former Heads of

RSD and Dr. S.M Lee, former Director, Safety Group were present to render their valuable suggestion and guidance to the programme.

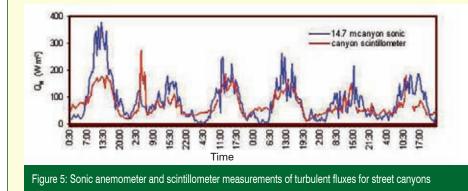
While emphasizing the importance of Fast Breeder Reactors for ensuring the power security of the country the enormous scope and depth for pursuing study in frontier fields and also for undertaking collaborative research is recognized especially in the context of the on-going research programme in the



field of atmospheric dispersion studies under Safety group. It was felt that while dispersion and diffusion in long distance transport and in complex terrain are the present day challenges, consideration must also be given for site specific terrain features. Advanced models are pointed to be more suitable from this perspective. The requirement of experimental validation of these models, incorporation of air flow around buildings, surface roughness on a micro scale was highlighted. The invited talks dealt with various aspects of wind flow modeling with particular reference to prediction of dispersion in a complex site like Kalpakkam with topics covering dispersion in calm condition, meso-scale models and real time data assimilation techniques.

The talks by experts included studies on flow field simulations with mesoscale models like RAMS, MM5, WRF for larger regions and with CFD based models such as FLUIDYNE PANIPR, ACRi ANSWER for medium to micro scale over the complex terrain. Studies of simulations on windflow and convective thunder storm prediction, the effect of water body on the frontal movement; specific case studies such





Dr.A.N.V.Satyanarayana, CORAL, IIT, Kharagpur presented the analysis of atmospheric boundary layer measurements using fast response sensors in urban street canyons and their importance in understanding dispersion in complex topography (Figure 5)

Dr. Amit Apte, CAM, TIFR, Bengaluru discussed the development of data assimilation module in atmospheric model using the Ensemble Kalman Filter.

Prof S.Ramakrishna presented the flow field simulations for Vizag complex terrain using MM5 model and the application of SODAR developed by Andhra University for observing the sea breeze, internal boundary layer at the coast (Figure 6).

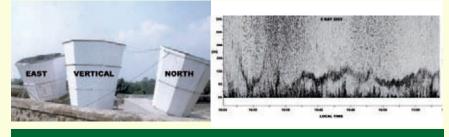
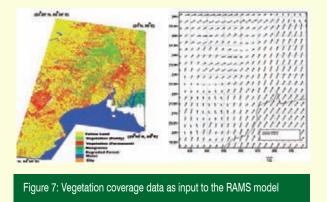


Figure 6: Monostatic Sodar at Andhra University showing sea breeze at Vizag coast on may 6, 2003

Dr.Debasish Lohar, Jadavpur University emphasized the necessity of representing the effects of vegetation and terrain sloping on mesoscale wind flow pattern through simulations using RAMS for a region in West Bengal (Figure. 7).



Dr. B.S.Murthy, IITM, Pune discussed the sea breeze and PBL simulations for a coastal site and their validation with experimental SODAR and Tether SONDE data sets (Figure 8).

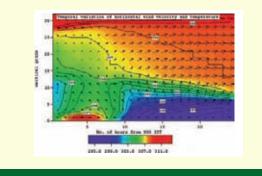


Figure 8: Simulated diurnal vertical profiles of wind and temperature

as Bhopal gas leak accident during a calm wind condition, sea breeze and atmospheric boundary layer at coastal sites, application of advanced data assimilation techniques like 3DVAR, 4DVAR using conventional and satellite based meteorological model observations for improvements were presented. The possibility for developing a data assimilation module in the atmospheric model with "Ensemble Kalman Filtering" was discussed. The advantages of high resolution vertical profile data obtained with indegenously developed SODAR and GP Sondes and their specific applications in turbulence measurements in atmospheric boundary layers at coastal sites were highlighted. A systematic analysis and estimation of atmospheric surface layer parameters using similarity relationships based on boundary layer data was proposed. The need for site specific non-meteorological data such as land use/ terrain and soil categories generated through remote sensing and GIS as an essential input in CFD and mesoscale models was recognized.

A brainstorming session was held with experts from DAE in the TDM to clarify and define the objectives of the Round Robin Exercise and to frame the modalities for pooling together the technical, manpower resources and expertise available with the participating institutions to get a meaningful result with in the short time frame of one year. It was decided that the goal of the Round Robin Exercise is to evolve a dispersion code for a region of interest in meso, medium and micro scales covering domains of 100, 10 km and an inner domain of 1 to 4 km and evolve simple schemes to initially model and validate the flow field and the atmospheric turbulence parameters.

The following points emerged from the two day deliberations with a roadmap to be followed for executing the Round Robin Exercise on a mission mode with clearly spelt out objectives.

- Emphasis is to be on rigorous comparison of models for wind field and other meteorological and turbulence parameters at the scales relevant to dispersion studies.
- A network of fast and conventional sensors in the above domains needs to be set up with a view to create a set of bench mark data in two to three months time. All the instruments available with participating groups would be pooled together.

- Fast response and other sensors must be located at source and receptor locations and the data sets have to be compared sufficient number of times. A detailed methodology for a meaningful and objective comparison would be formulated.
- ISRO, with whom there are ongoing collaboration projects, will be requested to augment the measurements with their state of art equipments. (AWS, MBLM, GPS Sonde etc.)
- The enormous data generated during the measurement campaign should be properly archived, quality checked, analyzed and programs should be developed for a discernable visual display.
- A comprehensive experimental field measurement campaign is scheduled for February to April 2010.

Under the Round Robin Exercise, well calibrated bench mark atmospheric data would be generated by deploying different platforms for measurement like AWS, SODAR, GPS Sondes, Met tower, portable masts at a number of locations in and around a small region of interest. All the measurements would be simultaneously made to provide a unique opportunity for all the research teams to come together and use the data for the goals of the Round Robin Exercise. The comparison of the wind flow would be preferably in time and spatial averaged quantities rather than point based. Along with the meteorological parameters the radiological data like Tritium-3 and Argon-41 would also be included for simultaneous measurements during the campaign and used as objective parameters for comparison. The Round Robin Exercise would be funded by the Board of Research in Nuclear Sciences (BRNS) as a major effort in supporting the academic and other research institutions in the field of safety research especially dispersion studies. The objective of the collaborative proposals would contain a short-term goal for licensing applications and long-term research goal. The short term studies would essentially provide site specific correction factors for existing codes taking into account the fumigation and building wake effects due to various specific features of Kalpakkam site.

> (Reported by K.M.Somayaji and colleagues, Radiological Safety Division, Safety Group)

Young Officer's FORUM

Source Subassembly for Fast Reactors

Source subassembly design for fast reactors is a very challenging task as it involves reactor physics, heat transfer, thermal-hydraulic and mechanical design aspects. Also, information on source subassembly design is not practically available for other fast reactors. Source subassembly design has been completed and salient features of the design are discussed below.

Need for external source

The reactor has to be monitored continuously during operation as well as during shutdown and start-up using neutron detectors located at core cover plate in control plug. During normal operation of the reactor, the neutron flux at this location is sufficient to obtain measurable count rates. However, during shutdown and fuel handling conditions, the shutdown count rate available at the detector location is only 0.3 counts per second (cps) as against the requirement of minimum shutdown count rate of 3 cps at any time as per stipulations of AERB. Hence to satisfy the requirements, it is essential to have an external source that can supplement the count rate needs. Towards this requirement, Sb₂O₂-Be (γ-n) type source is chosen for PFBR with the experience gained by its use in FBTR.

Location, life and number of source subassembly

Location and number of source subassembly is very important as they would displace some fuel/ blanket subassembly in the core. Fuel subassembly being displaced would result in penalty on the total power and hence an optimum position is arrived at. Three source subassemblies are located 120° apart symmetrically in the blanket region (8th ring) next to core-II fuel subassemblies in the PFBR core. The life of source subassembly is 4 cycles of operation and is governed by the limiting fluence of 80 dpa for the hexcan and the clad. Additionally, they remain in storage location for three cycles for decay and cooling. The number of source subassembly required is arrived at from the requirement of minimum shutdown count rate of 3 cps at the detector location after two months of shutdown. The variation of count rate versus shutdown period for different number of source subassemblies is shown in Figure 1. From the Figure, it is inferred that with two source subassemblies, count rate of 3.2 cps is Shri T. Rajkumar obtained his B.E. degree in Mechanical Engineering from Adhiyamaan Engineering College, Hosur in 2003. He is from 1st batch of IGCAR Training School and



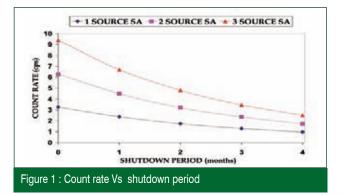
joined IGCAR as Scientific Officer (SO/C) in September 2007 and is working in Core Engineering Section, Nuclear Engineering Group.

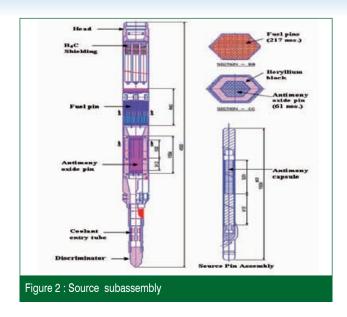
available after two months of shutdown, but at the time of replacement of source subassembly, there will be only one source subassembly in the reactor which is not sufficient to provide the necessary count rates. Hence there is a need to have a third source subassembly so that at the time of replacement, there will be effectively two source subassemblies in the reactor providing the shutdown count rate of 3.2 cps. Hence three numbers of source subassemblies are considered for PFBR.

Design criteria

The number of source subassembly should be less since more number of source subassemblies necessitates loss of more blanket subassemblies. Hence, based on the source volume requirement, the number of source subassembly is restricted to three and the source volume per subassembly is arrived as 455 cm³. The required source volume per subassembly is achieved by selecting suitable pin diameter, length and number of pins in a subassembly. The constraints being:

- The melting point of antimony oxide (655°C) as well as its thermal conductivity are very low. This restricts the pin diameter to be small since the centreline temperature of antimony oxide at 115% peak power under hotspot conditions shall not exceed its melting point.
- The source length shall be restricted between the bottom and middle levels of the active core region (500 mm max.) with a minimum length of 250 mm from active core bottom. This is to





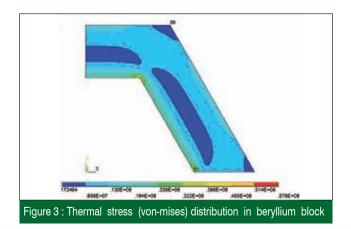
avoid the direct contribution of source neutrons to detector.

- The beryllium which surrounds antimony oxide should have minimum thickness of 20 mm on all sides to produce enough source neutrons. To meet this requirement, the number of pins should be less.
- The heat generation in source subassembly is very low when compared with the adjacent fuel subassembly. Hence coolant flow in the source subassembly should be such that the sodium temperature difference between the adjacent fuel subassembly and the source subassembly at the exit is less than 100°C from thermal striping considerations. Also, the coolant flow should respect the melting point of antimony oxide.

Hence, the requirement of source material volume, to accommodate within the standard subassembly geometry meeting the temperature limits is challenging and design incorporates appropriate engineering solutions to meet the above challenges.

Description of source subassembly

The source subassembly consists of sixty one pins



of antimony oxide surrounded by a hexagonal beryllium block of length 500 mm. The source volume in the pin starts exactly at the active core bottom level and it extends up to the middle of the core. Since the heat generation in source subassembly is very low as compared to the adjacent fuel subassembly, to avoid thermal striping in the control plug, short length fuel pins (217 numbers) are incorporated to increase heat generation in source subassembly which is a novel feature. Fuel pins in which the fuel column (mixed oxide fuel with 27.7% PuO₂) has a length of 275 mm and are supported above the source pins. The external features, head and axial shielding of source subassembly are identical to that of blanket subassembly.

Source pin assembly

Cast form of Sb₂O₃ is selected since it gives high density and thermal conductivity as compared to powder/sintered form. To have defect free casting of Sb₂O₃ pellets, an optimum length of 50 mm is chosen and is cast inside a SS 316 M clad of OD 5.1 mm and ID 4.36 mm. This capsule is seal welded with end plugs on both ends. Ten numbers of such capsules are stacked one over another in an outer clad tube (pin) of OD 6.6 mm and ID 5.7 mm and will be capped at both ends with another set of end plugs.

The melting point of Sb_2O_3 is low and also due to the low thermal conductivity of Sb_2O_3 and since the power generation is high, sodium is selected as the conducting medium between the capsules and the clad. The source pins are arranged in triangular pitch forming a hexagonal array. Coolant flow of 12 kg/s is required to respect the temperature limits. Satisfying all the design constraints, the antimony oxide pin is designed and the overall configuration of the source pin assembly is shown in Figure 2.

Beryllium block assembly

Beryllium is toxic and hence is housed in a helium filled leak tight container. Beryllium block assembly consists of beryllium block covered by outer and inner hexagonal sheaths welded with end plates at top and bottom. The swelling and thermo-mechanical analysis (Figure 3) of beryllium block assembly were carried out and the dimensions are arrived at.

Source subassembly design has been evolved incorporating suitable features addressing the design challenges and satisfying the design criteria.

> (Reported by T. Rajkumar, Reactor Components Division, NEG/REG)

Young Researcher's FORUM

Raman Spectroscopy of Nanostructured Materials

n recent years, semiconductor nanostructures have gained significant attention from many researchers due to their promising application in next-generation electronic, opto-electronic devices and solid state lasers. The size of nanostructure is large enough to maintain bulk crystalline structure; on the other hand, it is too small to retain the electronic and optical properties of bulk crystal. When the size of a nanostructure is comparable with the de Broglie wavelength of electrons, quantum confinement comes into picture thereby affects the opto-electronic properties of nanocrystal. Using advanced synthesis techniques, one can tune the size of nanocrystals to engineer their opto-electronic properties. In analogy with the quantum confinement effect of electrons and holes, phonons also exhibit confinement effect in small nanocrystals. Therefore, studies of phonons in nanocrystals are of interest both from fundamental and applications point of view. Raman spectroscopy has been used extensively to understand the confined phonons and their interaction with electrons in zero, one and two dimensional nanostructures including single atomic layer structures such as graphene. However, from the experimental point of view, the understanding of the size dependent Raman line shape of confined optical phonons in nanocrystals is far from complete; because of intrinsic and which can significantly modify extrinsic factors the actual Raman line shape. The intrinsic factors include size distribution, defects and substitutional disorder in nanocrystals. The extrinsic factors include temperature and stress. Stresses in nanocrystals arise when nanocrystals are synthesized inside a host matrix. Hence, it is worth examining the contribution of aforementioned effects to the Raman line shape.

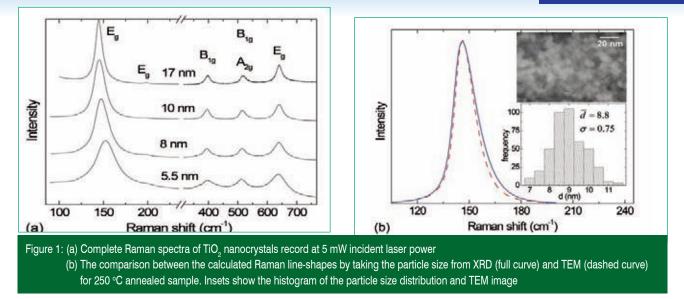
The present study can broadly be classified into three tasks. The first task is mainly focused on the confined optical phonons of zero dimensional Shri Satyaprakash Sahoo did his B. Sc. from Stewart Science College and M. Sc. in Physics from Ravenshaw College, Cuttack, Orissa. He joined IGCAR as Research Scholar in June 2005 and is pursuing Ph.D. on Raman study of nanostructured semiconductor materials, under the guidance of Dr. A. K. Arora.



nanocrystals/quantum dots. The emphasis is given on the contributions of defects, laser-induced local heating, substitutional disorder and stresses on phonon confinement. The second task emphasizes on the investigation of surface optical phonons arising from the diameter modulation of both one and two dimensional nanostructures. Finally, an attempt has been made to understand the effect of excitation energy on electron phonon interaction.

Different techniques are used to synthesize nanocrystals which include sol-gel method, chemical precipitation method, ion beam implantation and chemical vapor deposition. Conventional laser Raman spectrometer has been used to investigate the different phonon modes in nanocrystals.

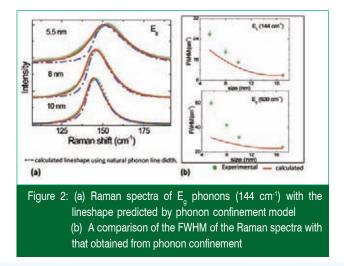
TiO, nanocrystals were synthesized by sol-gel method and as-synthesized powder was annealed at temperatures between 150 and 600°C to obtain nanocrystals of different sizes. The powder X-ray diffraction of these nanocrystals matches with the anatase phase of TiO,. Using Debye-Scherrer formula the sizes were calculated to be 5.5, 8, 10, and 16 nm for the samples annealed at 150, 250, 400 and 600°C, respectively. The average sizes estimated from TEM are found to be consistent with those calculated by XRD. The tetragonal structure of anatase has two formula units per primitive cell leading to six Raman active phonons: $3E_{q}$ (144, 196, and $639\,cm^{-1}$), $2B_{1a}$ (397 and 519 cm⁻¹) and $1A_{1g}$ (513 cm⁻¹). The Raman lineshapes of phonons of different symmetries; two E_{a} (144 and 639 cm⁻¹) modes and B_{1a} (397 cm⁻¹), mode have been analyzed for the first time quantitatively to distinguish between the contributions of laserinduced local heating, phonon confinement effects and defects to the line-broadening. A laser-induced local heating is found to cause significant line broadening and peak shift in TiO, nanocrystals of



different sizes. Hence all the measurements were done at lowest laser power of 5 mW and the obtained spectra are shown in Figure 1a. With decrease in particle size, the asymmetric broadening of the E_g and B_{1g} modes is found to be in opposite direction. The lineshapes of phonons of different symmetries have been analyzed using a phonon confinement model given by,

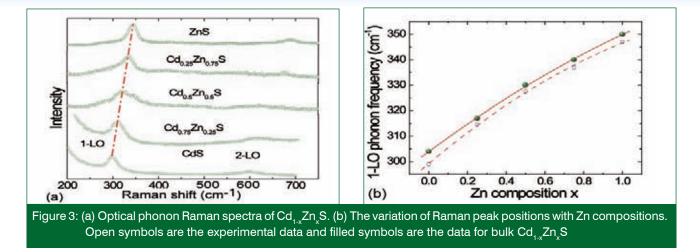
$$I(\omega,d) = \int \frac{|C(q,d)|^2}{[\omega - \omega(q)]^2 + (\Gamma_0/2)^2} d^3q \qquad (1)$$

where $\omega(q)$ is the phonon dispersion curve and Γ_0 is the natural linewidth of zone-center optical phonon in bulk anatase. C(q,d) is the Fourier transformation of the confinement function and Δ is the width of the dispersion curve of the optical phonon. It may be pointed out that Eq. (1) represents the lineshape for a given size. However, a wide distribution of particle size can significantly modify the Raman lineshape. The actual particle size distribution can be taken in to account by summing over the contributions from all the sizes. Figure 1b compares the total Raman



line broadening for the sample annealed at 250°C by taking the average size estimated from XRD and the size distribution obtained from TEM. The bright field TEM image and the size distribution are shown as inset in Figure 1b. The particle size is about 8.8 nm with a standard deviation of 0.75 nm which is consistent with XRD result. One can see from Figure 1b that both the calculated spectra differ marginally from each other due to narrow size distribution. All calculations are carried out by considering the sizes obtained by XRD.

The calculated confined phonon line shapes are compared with the measured Raman spectra for different particle sizes in Figure 2a. It is found that the data and calculated profiles do not match well for all the three phonons for smaller particle sizes, the disagreement being least for 144 cm⁻¹ E_a mode and largest for the 397 cm⁻¹ B_{1a} mode. The experimental line shapes for all the phonon modes are broader than the calculated profiles. In order to obtain reasonable agreement between the calculated and the measured spectra of 144 $\rm cm^{-1}~E_{_{\rm d}}$ mode, the Raman line shapes for nanocrystals of different sizes were recalculated using increased natural line widths and the calculated profiles are shown as full curves in Figure 2a. Similar analyses were also carried out for 397 cm⁻¹ B₁₀ and 639 cm⁻¹ E₀ modes. One can see that good fits to the data are possible using larger intrinsic widths. The full width at half maximum of the measured Raman spectra and those calculated using phonon confinement model for different modes are compared in Figure 2b as a function of particle size. One can see that for larger size particles there is



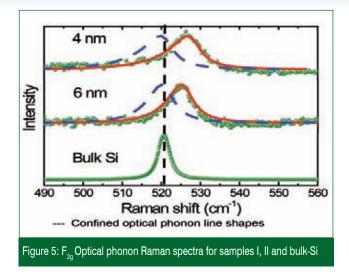
a good agreement between the measured linewidths and those predicted by the phonon confinement model. On the other hand, for small particles there is a significant difference between the two and one has to necessarily use larger intrinsic widths to get a good fit to the measured spectra.

In the present case, narrow size distribution of nanocrystals has no contribution on the extra line The possible reason for the extra broadening. broadening of the Raman lineshape could be the presence of defects in small nanocrystals. Assynthesized samples upon annealing at relatively lower temperature such as 150°C resulted in the formation of small nanocrystals. These nanocrystals are not expected to be free from defects. In order to examine annealing effect on the defect concentration, room temperature photoluminescence spectra of samples annealed at different temperatures were recorded. It is observed that defect related peaks at 2.3 and 2.98 eV disappear with increase in particle size. With increase in annealing temperature (increase in particle size), the defects are annealed out which indicates that smaller nanocrystals have large defect concentrations. The defects scatter phonons causing their decay and consequent decrease in life time. This results an increase in phonon line width. It is found that among the phonons studied in the present work, 397 cm⁻¹ B_{1a} and 639 cm⁻¹ E_{a} modes show much larger disagreement as compared to the 144 cm⁻¹ E_a mode. This suggests that these modes are more sensitive to the presence of defects as compared to the most intense 144 cm⁻¹ E_a mode. Hence, it can be concluded that observed Raman line shape for smaller nanocrystals shows larger disagreement with the calculated ones.

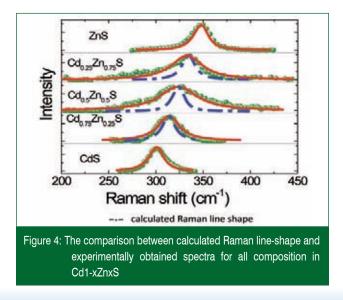
Phonons in nanocrystal of mixed crystal semiconductor are of special interest as the Raman lineshapes of these phonon modes are governed both by phonon confinement and substitutional disorder. Thus it is worth examining the relative contribution of these two effects to Raman line broadening. For this purpose, Cd, Zn S nanocrystals (x=0, 0.25, 0.5, 0.75 and 1) were synthesized at room temperature by chemical precipitation route in aqueous medium. The longitudinal optical (LO) phonons in free-standing mixed Cd, Zn S nanocrystals are investigated and Raman spectra are shown in Figure 3a. The longitudinal optical modes are found to appear at slightly lower frequency than those in the bulk mixed crystals and exhibit one mode behavior as shown in Figure 3b. Both the XRD and TEM suggest that the particle sizes of these mixed crystals are of nearly same size with a narrow size distribution. The 1-LO phonon line shape of each composition is analyzed using phonon confinement model. It is found that the calculated spectra match well with the data only for the end members, i.e., CdS and ZnS, whereas for the intermediate compositions the measured spectra are broader than the calculated one, the disagreement being maximum for x = 0.5. The good agreement between the measured and calculated spectra for the end members confirms that in pure CdS and ZnS nanocrystals the phonon confinement is the only mechanism of Raman line broadening. The departure of the calculated Raman line-shape from the data for the intermediate compositions suggests that the substitutional disorder also plays a significant role in determining the line width. We now attempt to quantify the relative contributions of phonon confinement and substitutional disorder to line broadening. In order to obtain reasonable

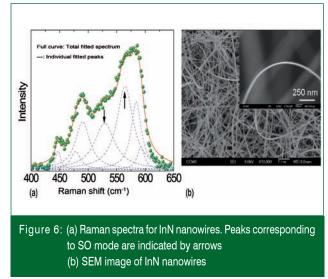
agreement between the calculated and the measured spectra of the mixed nanocrystals, the Raman line shape for the intermediate compositions were recalculated using increased natural line widths of 1-LO phonon and the calculated profiles are shown as full curves in Figure 4. Note that these are much higher than the value of 12 cm⁻¹ applicable for the pure compounds and represent the broadening arising from substitutional disorder. One can see that the measured linewidth increases with Zn substitution and reaches a maximum value for x = 0.5 and then starts decreasing with further Zn substitution. This is expected because the substitutional disorder is maximum for x = 0.5. On the other hand, the line broadening arising from phonon confinement decreases marginally and nearly linearly with the composition. The compositional dependence essentially arises due to variation in the phonon dispersion relation. It is found that the contribution from substitutional disorder to the line width is much more than that arising from the phonon confinement. Thus from the present quantitative line-shape analysis, it is possible to extract the contribution of different broadening mechanisms of the LO phonon line-shape in mixed nanocrystals.

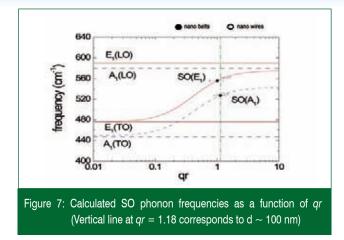
An attempt has also been made to understand the effect of stress on the phonon modes of nanocrystals. For this Si nanocrystals of different sizes embedded in sapphire were synthesized using ion-beam implantation. Confined acoustic and optical phonons in Si nanoclusters are investigated. The confined acoustic phonons are analyzed using complex frequency model to estimate the size of nanoclusters



and sizes are found to be 4 (sample I) and 6 (sample II) nm. Average size estimated from TEM shows a close agreement with the above sizes. The Raman spectra of F_{2a} optical phonon in Si nanocrystals show distinct peaks at 525.9 and 524.0 cm⁻¹ for samples I and II, respectively. The expected Raman spectra as calculated using phonon confinement model are also shown in Figure 5 as dashed curves. Note that except for the peak position, the calculated phonon line shapes for 4 and 6 nm particles match well with the observed Raman line shapes of samples I and II, respectively. The peak positions expected from phonon confinement model for 4 and 6 nm Si nanoparticles are 519 and 519.4 cm⁻¹, respectively; whereas the observed phonon peaks are found at 525.9 and 524 cm⁻¹ for samples I and II, respectively. This blue shift of the peak-centers of optical phonon can arise if the embedded Si-nanocrystals (nc-Si) experience compressive stress. The pressure exerted by the Al₂O₃ matrix on nc-Si can be obtained







from the blue shift of optical phonon frequency. For sample I (4 nm) and sample II (6 nm), the pressures are calculated to be 1.2 and 0.8 GPa, respectively. From the XRD pattern of these nanoparticles, shift in the peak position is also observed which suggests a compressive strain on the nanoparticles. The compressive stress develops due to the differences in the elastic constant and the thermal expansion coefficients of the particles and the host. Furthermore large particles are expected to have less stress as compared to small particles, because during the growth of larger particles the stress gets relieved by deforming the surrounding host.

In addition, Raman spectroscopic investigations of phonons in one dimensional nanostructures of InN, such as nanowires and nanobelts, were carried out. The wurtzite crystal structure of InN belongs to C_{ev} point group symmetry. A total of six Raman active modes are reported, which are $A_1(LO)$, $A_1(TO)$,

 $E_1(LO)$, E_1 (TO), E_2 (high) and E_2 (low) at 586, 447, 593, 476, 488 and 87 cm⁻¹, respectively. In polar crystals, surface optic (SO) modes are observed on the low frequency side of LO mode. In the present study, apart from the five Raman active modes expected between 400 and 650 cm⁻¹, two additional modes around 528 and 560 cm⁻¹ are found as shown in Figure 6a. The SEM images of nanowires are shown in Figure 6b. We examine the possibility of surface phonon being responsible for the new modes found for InN nanowires and nanobelts.

We calculate the frequencies of the SO phonon modes for nanostructured InN. The expression for the SO phonon frequency for a 1-D nanostructure is given by,

$$\omega_{SO}^2 = \omega_{TO}^2 + \frac{\omega_p^2}{\varepsilon_\infty + \varepsilon_m f(x)}$$
(2)

Where ω_{TO} is the frequency of TO phonon, ε_{o} and ε_{∞} and are the static and high frequency dielectric constant of the material and ε_{m} is the dielectric constant of the medium and ω_{p} is the screen ion plasma frequency. f(z) is given by $f(z) = [K_{\eta}(z)I_{0}(z)/I_{\eta}(z)K_{0}(z)]$, where I_{j} , and K_{j} are the modified Bessel functions. We have used 10.3 and 6.7 corresponding to ε_{o} and ε_{∞} , respectively, for InN. The dielectric constant of the medium (air) is taken as 1. Figure 7 shows the ω_{so} as a function of qr. For d ~100 nm, the value of qr turns out to be 1.18 and the corresponding calculated SO modes are found to be in agreement with the observed ones. Therefore, one may assign the modes at around 528 cm⁻¹ and 560 cm⁻¹ to SO modes with A_{1} and E_{1} characters, respectively. The

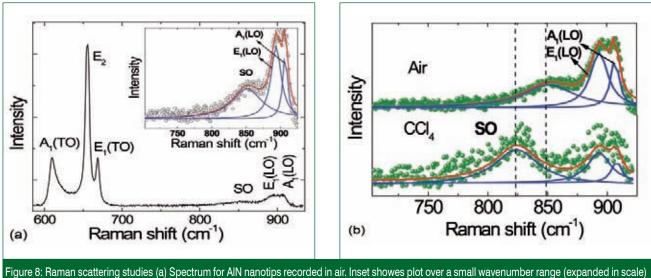
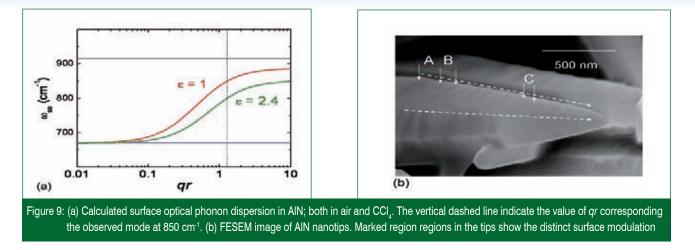


Figure 8: Raman scattering studies (a) Spectrum for AlN nanotips recorded in air. Inset showes plot over a small wavenumber range (expanded in scale (b) Plots showing comparison of the position of SO phonon peak in air and CCl₄ medium



broad nature of the SO phonon essentially arises due to the wide range of the nanowires and nanobelts diameter/dimension. The SO phonon dispersion largely depends on both the dielectric function of the semiconductor and that of the surrounding medium in contact. Taking this into account, typical Raman spectra for NWs in a higher dielectric medium (ε_m = 2.24 for CCl₄) are recorded and a clear red-shift ~4 cm⁻¹ for SO modes are observed. Hence, both the calculated and experimental results support our assignment of these peaks as SO modes.

Similar investigations of SO phonons in AIN nano tips were also carried out. Apart from the group theoretically allowed optical phonons, a new phonon mode at 850 cm⁻¹ has been observed for the first time as shown in Figure 8a. We have calculated the SO phonon dispersion for AIN nano tips using Eq. (2). In the calculated dispersion curve, the observed new peak at 850 cm⁻¹ has a corresponding $\chi = 1.2$ in air. In order to observe SO phonon on a perfect surface, the surface has to absorb the required phonon momentum. This can be achieved with the help of regular defects on the surface. We examine the surface of AIN using a high resolution FESEM, Figure 8b. One can see that each nano tip consists of steps of constantly reducing sizes along the length of nanotips. Typical analyses of the surface (as directed by two doted arrow) show that the steps are systematically decreasing along the growth direction. It is possible to calculate q for each plate by taking corresponding r and χ =1.2. From the q values for each steps the wavelengths ($\lambda = 2\pi/q$) of perturbation were calculated as shown in Figure 9. These values are in close agreement with the length of the steps, as indicated in Figure 8b. The observed new peak

shows a significant red shift in presence of higher dielectric medium (CCl₄). Hence, both the calculated and experimental results support our assignment of these peaks as SO modes.

Finally a wavelength dependent electron-phonon interaction in ZnO nanocrystal was investigated. Raman spectroscopic studies were carried out on ZnO nanoparticles for various photon energies. Intensities of E_1 -LO and E_2 modes exhibit large changes as a function of the excitation energy. This signifies substantially large contribution of Frohlich interaction to the Raman polarizability as compared to deformation potential close to the resonance. A comparison of the ratio of E_2 and E_1 -LO intensities with that of bulk suggests that the electron–phonon interaction for E_2 phonon decreases less rapidly than E_1 -LO phonon with a reduction in size.

In conclusion, Raman investigation of nanocrystals of zero dimensional structures have been investigated to understand the contribution of various factors like defects, substitutional disorder, stress to the total Raman line shape of confined optical phonons quantitatively. These effects must be taken in to account for the analysis of Raman line shape in nanocrystals. In one and two dimensional nanostructure of InN an AIN the surface optical phonons have been investigated and assigned for the first time. The origin of these surface modes is attributed to diameter modulation of these nanostructures.

> (Reported by Satyaprakash Sahoo, Condensed Matter Physics Division, MSG)

News and Events

Graduation Function of 3rd batch of BARC Training School at IGCAR



Dr. Baldev Raj, Director, IGCAR addressing the graduates along with Prof. S.K.Joshi, JNCASR Vikram Sarabhai Professor, National Physical Laboratory, New Delhi and other colleagues.

The third batch of Forty three Trainee Scientific Officers from the BARC Training School at IGCAR have successfully completed their training and were graduated in a special ceremony that took place on September 1, 2009 at the Sarabhai Auditorium, Homi Bhabha Building, IGCAR. Distinguished Academician, Prof. S.K.Joshi, JNCASR Vikram Sarabhai Professor, National Physical Laboratory, New Delhi was the Chief Guest. Dr.M. Sai Baba, Head, Strategic and Human Resources Planning Section and Head, BARC Training School at IGCAR welcomed the gathering. Dr.Baldev Raj, Distinguished Scientist and Director, IGCAR addressed the gathering. Prof.S.K.Joshi gave away the prestigious 'Homi Bhabha Prize' comprising of a medallion and books worth Rs.5000 to the meritorious toppers from all the disciplines. He also gave away the course completion certificates to all the graduates passing out. A few of the Trainee Scientific officers passing out, gave a feedback on their academic programme and their stay at hostel. A souvenir featuring the first year of the training programme at IGCAR was released by Prof.S.K.Joshi on this occasion and Dr. Baldev Raj received the first copy. Prof. S.K.Joshi gave a very inspiring and enlightening lecture to the gathering. Dr.Vidya Sundararajan, S&HRPS proposed the vote of thanks.



3rd Batch of Graduates of BARC Training School at IGCAR with the Chief Guest, Chairman, Director, Senior colleagues of the Centre and members of S&HRPS

(Reported by M. Sai Baba, S&HRPS)

Visit of Dignitaries

Shri D. P. Shrivastava, Ambassador of India to Czeck Republic, visited the Centre on July 10, 2009. He met Dr.Baldev Raj, Director, IGCAR and other senior colleagues of the Centre. He visited the Fast Breeder Test Reactor and construction site of PFBR at BHAVINI.



Shri D.P.Shrivastava, Ambassador of India to Czeck Republic with Dr.Baldev Raj, Director.IGCAR



Prof. M. M. Sharma, Emeritus Professor and former Director, University Institute of Chemical Technology, Mumbai with Dr. Baldev Raj, Director, IGCAR along with other members of the "Peer Committee in Chemical Sciences" and senior colleagues of the Centre

Prof. M. M. Sharma, Emeritus Professor and former Director, University Institute of Chemical Technology, Mumbai visited the Centre during August 3-4, 2009. He chaired the "Peer Review Committee in Chemical Sciences". Prof. M. M. Sharma delivered the lecture on "The exciting and rewarding world of Chemistry and Chemical Engineering" in the "Eminent Lecture Series" organized as a part of commemorative celebrations of birth Centenary of Dr. Homi Jehangir Bhabha. Prof. M. M. Sharma visited various laboratories of the Centre.

Prof. Siegfried S. Hecker, Director Emeritus, Los Alamos National Laboratory, USA visited the Centre on September 24, 2009. He delivered a lecture on "Plutonium: The promise, peril and puzzle" as part of eminent Prof. lecture series. Hecker also visited the Fast Breeder Test Reactor, Laboratories in Materials Science and Metallurgy & Materials Groups and also the construction site of PFBR at BHAVINI.



Prof. Siegfried S.Hecker, Director Emeritus, Los Alamos National Laboratory, USA with Dr.Baldev Raj, Director, IGCAR and other colleagues of the Centre with Research Scholars and TSO's of BARC Training School at IGCAR

Visit of Dignitaries

Dr. Mohammed El-Baradei, *Director General, IAEA, Vienna* visited the Centre during September 27-28, 2009. He met Dr. Baldev Raj, Director, IGCAR and other DAC members. He visited the Fast Breeder Test Reactor, Hot cells and laboratories in the Non-Destructive Evaluation Division, construction site of PFBR at BHAVINI, Nuclear Desalination Development Plant and Safety Research Institute of AERB. He was also accompanied by Shri Sourabh Kumar, Ambassador to IAEA, Vienna during his visits.



Dr. Mohammed El-Baradei, Director General, IAEA, Vienna with Dr.Baldev Raj, Director, IGCAR



Prof.Thomas Fanghanel, Director, Institute for Transuranium Elements, Joint Research Centre, European Commission during his visit to Chemistry Group along with his colleague Dr.Frank Wastin and senior colleagues of the Centre

Prof. Thomas Fanghanel, *Director, Institute* for Transuranium Elements, Joint Research Centre, European Commission visited the Centre during September 27-28, 2009. During his visit, he was taken around the Fast Breeder Test Reactor, laboratories in the Non-Destructive Evaluation Division, laboratories in Materials Science Group and Chemistry Group. He also visited the construction site of PFBR at BHAVINI. Prof. Fanghanel delivered a Lecture on "Closing the Fuel Cycle for a Sustainable Future Nuclear Energy" as part of "eminent lecture series".

Dr.Jacques Bouchard, *Special Advisor* to Chairman, CEA and Chairman, GIF,CEA visited the Centre during September 27-28, 2009. During his visit, he was taken around the Fast Breeder Test Reactor, laboratories in the Non-Destructive Evaluation Division, Fast Reactor Technology Group, Safety Group and Structural Mechanics Laboratory. He also visited the construction site of PFBR at BHAVINI. Dr. Bouchard delivered the lecture on the topic "Nuclear Energy and Sustainable Development" as part of the "Eminent Lecture Series".



Dr. Jacques Bouchard, Special Advisor to Chairman, CEA and Chairman, GIF,CEA during visit to Structural Mechanics Laboratory along with his colleague Dr. Sunil Felix and other senior colleagues of the Centre

Forthcoming Meetings / Conferences



23rd International Conference on Surface Modification Technologies (SMT 23) November 2-5, 2009

As part of the birth centenary year of Dr. Homi Bhabha, the 23rd International Conference on Surface Modification Technologies (SMT 23) is being organized at IGCAR, Kalpakkam during November 2-5, 2009. It is organised by The Indian Institute of Metals, Kalpakkam Chapter, Indira Gandhi Centre for Atomic Research, Kalpakkam, CII - LM Thapar - Centre for Competitiveness for Surface Modification Engineers Confederation of Indian Industry.

The conference will be held at the GRT Temple Bay, Mamallapuram, Chennai. The objective of this meeting is to provide a forum for open discussion amongst scientists and engineers from different fields such as physics, chemistry, engineering and on the enormous potential for the adaptation of surface science and engineering. Several technical sessions focusing on the state of the art developments in surface science and engineering with keynote and invited presentations by eminent professionals in the field are planned.

Aim & Scope:

- * To create an interactive forum for multi-disciplinary discussion and to encourage interactions between scientists/engineers and personnel from industrial, research and academic organizations
- * To identify new processes and frontier areas of research in traditional and advanced surface modification techniques and analysis
- * The conference will speculate on future trends relating to surface modification and analysis

Research papers and participation from industries are being solicited in the following areas:

- PVD, CVD, DLC, biomedical, polymer, high temperature coatings.
- Electroplating, Electroless plating, Anodizing.
- Galvanising, Hard-facing, Weld cladding and overlay, nitriding and organic and chemical conversion coatings.
- Plasma, Ion implanation, Electron Beam and Laser based coatings.
- Thin and thick films preparation and characterization and Nanotechnologies.
- Surface Analysis and Investigations using Optical microscopy, SEM, TEM, XRD, EPMA, XPS, AES, SIMS, NDT techniques etc.
- Surface electrochemistry and corrosion of coatings
- Functional testing of coatings
- Application of coatings in industrial setting to include aerospace, automotive, textile, biomedical and energy
- Surface engineering phenomenon properties applications

Important Dates:

Abstract Submission	: June 01, 2009
Acceptance of abstract	: June 30, 2009
Submission of full text	: August 30, 2009
Final Registration	: October 10, 2009

Address for Correspondence:

Dr. U. Kamachi Mudali Convenor, SMT 23 Head, CSTS-RPM, CSTD Metallurgy and Materials Group Indira Gandhi Centre for Atomic Research Kalpakkam 603 102, Tamil Nadu, India Tel:+91-44-27480805 / 27480121 / 27480500. Extn. 22794 Fax: +91-44-27480301 E-mail : kamachi@igcar.gov.in

Forthcoming Meetings / Conferences



Scientific Information Resource Division (SIRD), formerly Library and Information Services, Indira Gandhi Centre for Atomic Research(IGCAR), Kalpakkam and Madras Library Association -Kalpakkam Chapter(MALA-KC) have been conducting a series of conferences in Recent Advances in Information Science and Technology (READIT).

The Conference and Tutorial will be held at IGCAR, Kalpakkam, which is located 75 Km south of Chennai, the Capital of Tamil Nadu. It is also 10 km south of Mamallapuram, a fabulous South Indian tourist spot which is famous for architecture and sculpture skills of Pallava Dynasty. Kalpakkam is well connected by road and situated in the middle of Chennai to Pondicherry ECR scenic beauty highway and surrounded by temple cities like Kancheepuram & Thirukazhukundram and Vedanthangal bird sanctuary

Objective:

READIT 2009 targets professionals in the field of IT, Library & Knowledge Management to provide a forum for discussion and knowledge transfer in the field of semantic web technologies and application of the same in representing the organizational knowledge. The topics related to knowledge representation in digital library through semantic web, open source solution and strategies, standards, protocols and language used for knowledge representation would be addressed in detail.

A Pre-Conference Tutorial is also being arranged with the theme of "Digital Repository Creation and Preservation Management On December 28, 2009".

The conference will consist of invited talks and contributed papers in the following areas:

- Digital Library Infrastructure Development
- Semantic web technologies for Digital Libraries
- Digital Resource Organization & Discovery
- · Federated Search, Interoperability and Crosswalks
- Vocabulary and Taxonomy Development
- Knowledge Organization and Semantic Information Retrieval
- Open Source Solutions & Library 2.0
- Knowledge Management Practices in Library & Information Centres

Important Dates:

Pre-Registration (with Abstracts)	: November 16, 2009
Intimation of Acceptance	: November 22, 2009
Receipt of completed papers	: November 30, 2009
Acceptance of full papers	: December 7, 2009
Last date for Registration	: December 15, 2009

Address for Correspondence.

Dr. M. Sai Baba Convenor, Organising Committee, READIT-2009, Head, Scientific Information Resource Division, Indira Gandhi Centre for Atomic Research, Kalpakkam – 603 102, Tamil Nadu Phone: +91 44 27480281; Fax: +91 44 27480096; E-mail: readit@igcar.gov.in URL: http://library.igcar.gov.in/readit2009/readit2009.html

Forthcoming Meetings / Conferences



20th Annual Conference of Indian Nuclear Society (INSAC-2009) January 4-6, 2010

The 20th INS Annual Conference on Materials and Manufacturing in Nuclear Industry (INSAC-2009) is being jointly organized by Indian Nuclear Society, Indira Gandhi Centre for Atomic Research and Bharatiya Nabhikiya Vidyut Nigam Limited (BHAVINI).

The conference will be held at The Convention Centre, The Chennai Trade Centre, Chennai, Tamil Nadu, India. INSAC-2009 aims at creating a platform for the Indian and foreign industries to converge and share their experiences as well as the challenges in meeting the nuclear standards in areas of materials development and manufacturing. The conference also provides an opportunity for the Nuclear Societies from various parts of World to discuss and open up collaborative ventures in the area of nuclear science and technology.

Topics to be covered

- Materials properties
- Materials selection
- Manufacturing processesconversion coating.
- Heat treatment
- Welding science & technology
- Concurrent engineering
- CAD/CAM, Near-Net-shape
- Quality assurance
- Special materials for nuclear components
- Automation & robotics in manufacturing
- Advanced materials and coatings

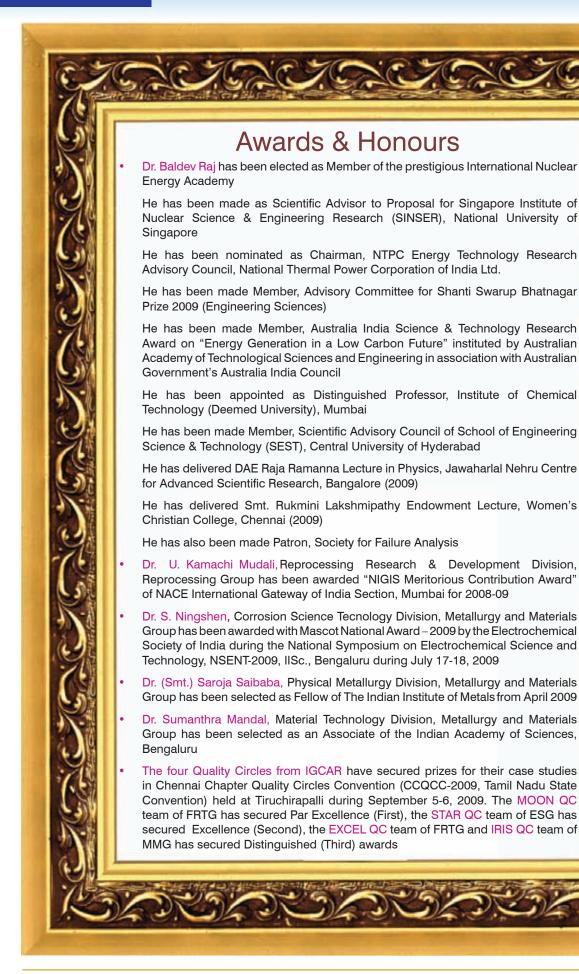
- Manufacturing of large components
- Rapid prototyping
- Codal and regulatory aspects
- Modeling, Simulation and Intelligent Manufacturing
- Plant layout, Product development and Manufacturing
 Management
- Rapid prototyping and Concurrent engineering
- Manufacturing innovations and Global trends in manufacturing
- Human resource development, IPRs and Knowledge management

Important Dates:

Abstract Submission	: October 01, 2009
Intimation of Acceptance (oral/poster)	: October 15, 2009
Submission of Paper	: November 30, 2009
Early bird registration incentive	: November 01, 2009
Deadline for registration	: December 15, 2009
Exhibition / Sponsors / Advertisement	: December 26, 2009

Address for Correspondence:

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