REPORT OF

US-India Workshop on

Nanotechnology: Issues in Interdisciplinary Research and Education (Aug. 11-13; 2004; at IISc Bangalore)

By

National Nanotechnology Infrastructure Network (NNIN)
and
Indian Institute of Science (IISc)

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Executive Summary

The second[1] of the Joint US-India Workshop entitled "Nanotechnology: Issues in Interdisciplinary Research and Education" took place at the Indian Institute of Science campus (Bangalore, India) from Aug. 11 through 13, 2004. The workshop was sponsored by National Science Foundation, Department of Science and Technology under its programme on Nano Science and technology Initiative, and the US-India Science & Technology Forum. Additional support was provided by the Jawaharlal Nehru Center for Advanced Research.

The focus of the workshop was on identifying the key needs and suggesting possible approaches for incorporating in undergraduate and graduate education the advances that are being made in the broad interdisciplinary area of nanoscale science and engineering. Through a discussion of the advanced and promising directions of research, the university educational imperatives, human resource needs, and the development needs of India and US, the workshop also explored the broader principles that any proposed changes should keep in mind.

The workshop brought together 12 technical speakers/participants from United States, from academia and industry, representing the diverse disciplines of science and engineering at the small dimensions. There were 14 technical speakers/participants from India, representing academia, industry, and national laboratories. Many of the major institutions of US and India were represented. The individuals from these institutions provided a diversity of opinions representing their discipline-centric and institution-centric backgrounds. In addition, the diversity of cultural backgrounds also provided unique perspectives.

The workshop was also attended by a large group (at times exceeding hundred) of graduate students, teaching college instructors, industry observers, and representatives from National Science Foundation and other interested and related Indian agencies.

The workshop identified the guiding principles that should determine the changes:

- an undergraduate education should provide a broad and rigorous core education that prepares the student to be analytical and rapidly trainable for active technical contributions in design and manufacturing based on the science and engineering areas
- a graduate education should have a rigorous, complete and advanced technical focus, drawing on the current knowledge and that makes the student an independent thinker and problem solver. Research is the central thrust in graduate education in order to provide the student with the capability to ask the appropriate questions and find the answers for theoretical and experimental directions.

Nanoscale science and engineering, unlike most of the previous major developments in new technical directions, is characterized by its inter-disciplinarity. It draws on the different engineering disciplines, physics, chemistry, biology, materials sciences, etc. to bring their experimental and theoretical tools and techniques together. The ability to form nano-scale structures by assembling from atoms and molecules up, and to precisely define and connect and

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[1] The first workshop took place at the University of California at Santa Barbara Campus. See S. Tiwari and K. Padmanabhan, Report and Digest of the Joint US-India Workshop on Nanotechnology, Nov. 7-8 (2001)

interface them with the macroscopic world make the multitude of new and major accomplishments possible across sciences and engineering. This inter-disciplinarity poses a key challenge in positing how best to incorporate the knowledge into traditional pedagogy or education.

The principal observations and recommendations of the workshop are the following:

- Undergraduate education should remain focused on the breadth and rigorousness of a core curriculum that emphasizes the underlying knowledge of physics, chemistry, mathematics, and increasingly in biology, followed by a selection of courses that lead to a more rigorous technical direction. Exposing students to the methods and key ideas of the scientific process are critical. This broad education, with a technical focus, is critical to their becoming successful practitioners who may not necessarily pursue advanced degrees.
    - Biology is increasingly connected to the physical sciences and engineering. The ability for a student to take at least one course in biology as an option would provide a more complete education than is currently provided.
    - Nanotechnology is not a discipline; it is an inter-disciplinary area with significant underpinnings in engineering disciplines, physics, chemistry, biology, materials sciences, etc. Undergraduate students need exposure to this area, both for the knowledge of the major current technical questions and directions and on how it connects to the core education. Furthermore, nanotechnology can be used as a vehicle to excite and motivate students to purse careers in science and engineering. At least two mechanisms for incorporating this idea are:
        - an evolutionary change of course content for a variety of the classes so that they reflect problems and approaches of the nano-scale, and
        - offering of elective courses – such as introductory-level freshman courses that excite and motivate the students to want to take related advanced courses in subsequent years.
    - The participants were unanimous in their opinion that nanotechnology is not an area for a new department, nor yet an area where a degree needs to be granted.
- Graduate education, with its advanced technical focus and goal of making the student an independent thinker and problem solver, poses an interesting challenge for the interdisciplinary nanotechnology area since the strength of the underlying disciplines must be maintained.
    - Quantum mechanics, thermodynamics/statistical mechanics (i.e., molecular thermodynamics), materials science, biology, chemistry, systems engineering, and engineering as dictated by design, are all key elements of an education that the student must be able to draw on. It is critical that the students receive education in

the related areas through approaches and instruction by faculty that connect to the science and engineering of the condensed state[2].

- Nanotechnology-oriented course offerings should draw on this knowledge to provide strong inter-disciplinary strength. Individual faculty members are not likely to be able to provide this inter-disciplinary breadth due to their discipline-specific focus.
  - A team approach (multiple faculty members across departments) to interdisciplinary teaching can provide a balanced method towards a more complete inter-disciplinary student education in nanotechnology that still assures that the underlying discipline-specific strengths are imparted.
  - New textbooks that can draw on modern computing and web-based resources that help connect the disciplines, are needed for effective instruction of a large group. Most universities are not likely to be able to draw on the multiple faculty members from different disciplines that are needed for effective teaching.

[2] Instances where quantum mechanics taught by a cosmologist/string theorist leaving the connection to the condensed state weak was one of the commonly sited example, as was thermodynamics connected to steam tables rather than the interesting problems of the small.

Introduction:

Nanotechnology is a key area of inter-disciplinary research whose discoveries and inventions are likely to have strong commercial and societal impact. Electronics, materials and coatings, and catalysis are areas where the commercial impact is already very significant, and biotechnologies, mechanical technologies, and other areas are likely to have significant growth in the coming years. Developing and training a knowledgeable work force consistent with the objectives of university education is a critical issue. This subject requires careful thought that balances the broader discipline-specific educational goals with the need of the technical strengths engendered by this important inter-disciplinary area.

Unlike in the past, where significant areas with economic impact have developed around core disciplinary areas, nanotechnology is distinguishable by its inter-disciplinary nature and the preponderance of research and technical innovations at the boundaries of science and engineering.

The workshop drew on these specific characteristics and focused on the educational needs through a dialog that was organized around the following principal topics:

- Key research ideas
- Underlying interdisciplinary aspects of the research
- Key issues of the interdisciplinary research and effective mechanisms for the pursuit of research
- Undergraduate and graduate teaching that addresses interdisciplinary research needs.

Workshop Participants:

Twelve key academic and industrial researchers from United States who are active in nanoscale science and engineering participated together with a larger group from India. The presenters from the Indian group consisted of representatives from academia, federal research laboratories, and industry. In addition a large contingent, exceeding hundred, of graduate students and teachers from other teaching and research universities and small colleges attended and participated in the deliberations of the workshop.

Appendix A lists the US and Indian speakers at the workshop.

Workshop Organization:

The technical sessions of the workshop were organized along discipline-oriented themes. This allowed a collection of talks that connected research to education to be followed by a discussion session where questions revolving around the theme could be discussed along with specific questions raised by the presentation. There were a total of 9 technical sessions that addressed characterization, physical phenomena of the small-scale, chemistry-based approaches, electronics issues, biology, materials, modeling and simulation, etc. The research areas encompassed by these talks included: electronics, sensors and nanotubes, optics, materials and coatings, surfaces and interfaces, modeling and predictive simulations, self-assembly and supramolecular chemistry, biotechnology and bioengineering, and the educational needs in these areas.

The introductory session of the workshop outlined the objectives of the workshop and included welcoming remarks from the head of the Indian Institute of Sciences (Prof. G. P. Mehta) and the Jawaharlal Nehru Center for Advanced Research (Dr. M. R. Rao). Dr. Rajinder Khosla and Dr. Usha Varshney from National Science Foundation provided a perspective of NSF and the legislative perspective of the Nanotechnology initiative.

Appendix B provides the abstracts of the presentations in a short form.

A CD and a limited number of digests with printed copies of the workshop talks are available from the workshop organizers and the presentations are accessible through www.nnin.org.

Figure 1: Snap-shots from the workshop. The US attendees are in the photograph on the left; the middle photograph shows the starting session (Prof. K. Chattopadhyaya spealing, Dr. R. Khosla of NSF, Prof. M.R.S. Rao who is President of Jawaharlal Nehru Center for Advanced Scientific Research, Prof. G. Mehta, who is Director of Indian Institute of Science, Dr. U. Varshney of NSF, and Prof. S. Tiwari. The photograph on the right is from a gathering at the workshop. Events at the workshop were hosted by Veeco and Icon Analytical.

Workshop Deliberations

The large-scale use of nanotechnology in society depends strongly on the successful transition from science to engineering to commercialization. Interdisciplinary research that leads to a successful vetting of ideas, education that supports the development of skilled researchers with diverse technical backgrounds and, ultimately, the transition of the two together into the marketplace are critical for success of nanotechnology.

Interest in nanotechnology stems from the modern ability to physically structure and chemically synthesize materials at the nanoscale with precision and with useful robustness, and as a result, has led to numerous advances in our understanding of fundamental physical phenomena. It has also resulted in the preliminary demonstration of applications that exploit these exceptional properties in exciting new ways. Potentially, nanotechnology allows the creation of materials and complex physical, chemical, and biological systems with unique properties dictated purely by design. The impact of this capability is vast. It will result in the creation of more powerful computing devices that function at lower power allowing the creation of more advanced information appliances and communications equipment. It will facilitate the development of energy efficient lighting and more efficient energy storage devices. It will enhance the effectiveness of catalysis processes. It will enhance the mechanical properties of materials by providing greater strength, durability and ruggedness and result in the development of new composite materials. Lastly, it will increase our understanding of fundamental molecular scale biological processes.

Harnessing these successes so that the society can benefit from their significant impact requires that the span of the effort – from scientific study to engineering application and effective education - is judiciously traversed. The transition from discovery to a practical or even potentially practical device or process is a long one. Tools and methods are critical, as are the foundations in reproducibility and control of properties, engineering control, manufacturability, cost, and scalability. Tools for fabrication, visualization, and characterization, as well as methods and standards to assure repeatability and accuracy of fabrication and analysis, and the connection of various techniques to making a well-engineered system with the desired properties are critical. Our understanding of the connections between the techniques, usually derived from different disciplines, and how they connect together for an engineering application are incomplete.

The talks of the work shop addressed the technical connections and the speakers provided their perspective on educational needs, and in many cases connected it to educational infrastructure. In optics, the technical discussions revolved around self-assembled quantum dots, photonic bandgap structures, and examples of use of opals to achieve 3D photonic bandgaps. A number of talks discussed nanotubes, their properties, and in particular their characteristics as sensors – flow sensors e.g. In electronics, the discussions revolved around the limits of dimensional scaling and key issues in design, architecture and technology that need to be addressed for continuation of progress. In molecular electronics, the discussions addressed issues of properties needed, reproducibility, interconnectivity and architectures. In chemistry, particularly at its interface with biology, a number of interesting approaches to use of biological processes for nanoparticle creation and contamination clean-up were discussed along with discussions of synthesis, Langmuir-Blodgett films, etc. Characterization was a particularly strong theme in the talks, with a number of talks discussing the need to understand what one creates, and the rigorous knowledge that this characterization requires. In physics, multi-scale phenomena, noise, different spectroscopies of small structures, and ultra-sensitive measurements were key areas of discussion.

The final session of the workshop integrated the earlier theme-based discussions on to education and educational infrastructure, its social context and human resource needs. The workshop participants strongly endorsed the goal of undergraduate education as a broad education with a rigorous core curriculum. The core curriculum needs to emphasize the underlying knowledge of physics, chemistry, mathematics, and increasingly biology. As an undergraduate student advances to the final years, the selection of courses gets more technically focused. Throughout this education, exposing students to the techniques and key thoughts of the scientific process are critical. This broad education, with a technical focus, is critical to becoming a successful practitioner. Most undergraduate students do not go on to receive advanced education, and are also likely to follow career paths that take them to technical areas that are distinctly different from areas that they emphasized in their education. In the coming years, biology is likely to become increasingly important. Most Indian students who follow an educational path in physical sciences and engineering, do not receive education in biology beyond the 10'th grade. The ability for a student to take at least one course in biology as an option would provide a more complete education than currently provided.

The workshop participants strongly supported the presentation of exciting nanotechnology-oriented content to students in the undergraduate curriculum, but also strongly felt that nanotechnology is not a discipline. Nanotechnology is an inter-disciplinary area with significant underpinnings in engineering disciplines, physics, chemistry, biology, materials sciences, etc. Undergraduate students need exposure to this area, both for the knowledge of the major current technical questions and directions and how they connect to the core education, as well as to excite the students. Two mechanisms are being suggested for incorporating this idea. The first is through evolutionary changes of course content of the variety of classes that reflects problems and approaches of the nano-scale. The second is the offering of elective courses – such as introduction at freshman level to excite the students and in subsequent years. The participants were unanimous that nanotechnology is not an area for a new department nor yet an area where a degree needs to be granted. For graduate education, a thorough advanced technical focus is vital. The education must also make the student independent thinkers, i.e., capable of asking the appropriate questions and finding answers. The interdisciplinarity of nanotechnology provides an interesting challenge since the strength of the underlying disciplines must be maintained. There was considerable discussion regarding the changes that have come about in teaching (or lack thereof) of quantum mechanics, electromagnetics, thermodynamics, etc. as a result of the pressures of course loads, and availability of faculty. These are core subjects, and for broader knowledge in nanotechnology, quantum mechanics, thermodynamics, materials science, biology, chemistry, systems engineering perspective, engineering as dictated by design, are all key foundations that the student must be able to draw on. It is critical that the students receive education in the related areas through approaches and faculty that connect to the science and engineering of the condensed state[3]. The workshop participants also strongly felt that characterization on nanostructures is a particularly challenging task and that there is a need for increased attention in this area in the curriculum.

The workshop participants felt that the nanotechnology-oriented course offerings should focus on the strong interdisciplinary strength. Individual faculty are not likely to be capable of providing interdisciplinary strength due to their discipline-specific strengths. A team approach (multiple faculty members across departments) to interdisciplinary teaching can provide a balanced method towards a more complete inter-disciplinary student education in nanotechnology that still assures the underlying discipline strengths education. Similar to the undergraduate education, the unanimous opinion of the participants was that nanotechnology is not an area for a new department nor yet an area where a degree needs to be granted.

[3] Instances where quantum mechanics taught by a cosmologist/string theorist leaving the connection to the condensed state weak was one of the commonly sited example, as was thermodynamics connected to steam tables rather than the interesting problems of the small.

A bit of discussion also revolved around the educational material needed. A strong case was made that new textbooks for interdisciplinary education are required. Creation of these textbooks can draw on new techniques that have been developed in the past many years. As an example these textbooks, written my multiple authors who come from different disciplines, can be strongly connected to modeling, simulation and visualization tools, and for their critical discussion, choose the new problems of nano-scale.

Recommendations:

With the above discussion as a perspective, the workshop makes the following recommendations:

- The discipline based strengths of education provided through core courses in physics, chemistry, and mathematics should not be compromised in any changes made. With the increased importance of biology, perhaps initially an elective option should be made available to undergraduate students.
- Undergraduate students should be encouraged towards the nanoscale science and engineering area through optional courses that bring about the interdisciplinary excitement of nanotechnology, but these courses should be strongly founded on the core disciplines.
- Experimental components in education are very necessary for completeness of education and courses should include these as appropriate.
- In graduate education, educational changes should make sure that quantum mechanics, statistical/molecular thermodynamics, etc. are taught in an appropriate manner that connections to the condensed state are maintained.
- Multidisciplinary nanotechnology courses will require multidisciplinary teaching. Team teaching, drawing on faculty from multiple departments, may best address this need. Effective teaching will require development of new text-books that draw on modern techniques that connect the content to scientific computation.
- Characterization should be incorporated as a key ingredient in the graduate teaching since nanoscale structures usually require very advanced techniques.
- Applications of nanotechnology are generally complex systems. Systems-level thinking is usually not an element in graduate engineering education. There is need for bringing systems-level techniques, similar to characterization, to nanotechnology education.
- Nanotechnology is interdisciplinary and not a discipline in itself. It is strongly connected to specific disciplines – physics, chemistry, biology, one of the engineering disciplines. All these disciplines are a focus of departments and degrees at academic institutions. Nanotechnology as an inter-departmental discipline has not yet progressed to a point similar to, e.g., bioengineering, where programs and departments exist. Granting degrees in nanotechnology is currently not recommended nor is creation of departments.

Acknowledgements

The success of the workshop resulted from a very broad effort including the enthusiastic participation of the attendees. For financial support, National Science Foundation, Department of Science and Technology, and US-India Forum on Science and Technology are gratefully acknowledged. The support of Dr. R. Khosla, Dr. M. Lueck, and Dr. R. Baheti at NSF, Dr. M. Cheetham at US-India Forum on Science and Technology, and Prof. CNR Rao at JNCAR were critical to the success of the workshop. A special word of appreciation to Prof. G.U.Kulkarni of JNCAR and Prof. Rudra Pratap of IISc for their help in organizational aspects. Logistical supports provided by Mrs. S.Rama and Mrs. Ranjitha at IISc were indispensable in bringing about a focused event.

Appendix A

US Speakers and Participants:

Prof. J. Silcox, Department of Applied and Engineering Physics, Cornell University

Prof. V. Dravid, Department of Materials Science, Northwestern University

Prof. A. Gopinath, Department of Electrical Engineering, University of Minnesota

Prof. S. Tiwari, Department of Electrical & Computer Engineering, Cornell University

Dr. P. Solomon, IBM Research Division

Prof. K. Saraswat, Department of Electrical Engineering, Stanford University

Prof. M. Rodwell, Department of Electrical Engineering, University of California/ Santa Barbara

Prof. M. Sapalle, Department of Mechanical Engineering, Iowa State University

Prof. V. Misra, Department of Electrical Engineering, North Carolina State University

Prof. S. Garde, Department of Chemical and Biological Engineering, Rensselaer Polytechnic Institute

Prof. E. Kaxiras, Department of Physics, Harvard University

NSF Participants:

Dr. Usha Varshney, National Science Foundation

Dr. Rajinder Khosla, National Science Foundation

Dr. V. Rao, National Science Foundation

Indian Speakers and Participants:

Prof. D. Chakravorty, Indian Association for the Cultivation of Science, Kolkata

Prof. A. K. Sood, Department of Physics, Indian Institute of Science

Prof. Santanu Bhattacharya, Department of Organic Chemistry, Indian Institute of Science

Dr. Murali Sastry, Nanoscience Group, Materials Chemistry Division, National Chemical Laboratory

Prof. D.D. Sarma, Solid State and Structural Chemistry Unit, Indian Institute of Science

Prof. V.Ramgopal Rao, Department of Electrical Engineering, Indian Institute of Technology, Mumbai

Dr. Pushan Ayyub, Department of Condensed Matter Physics & Materials Science, Tata Institute of Fundamental Research, Mumbai

Prof. S. K. Biswas, Department of Mechanical Engineering, Indian Institute of Science

Dr. G.V.Shivashankar, National Center for Biological Sciences, TIFR-Bangalore & Raman Research Institute

Dr. Milan K. Sanyal, Surface Physics Division, Saha Institute of Nuclear Physics, Kolkata

Dr. A.K.Raychaudhuri, S.N.Bose National Centre for Basic Sciences, Kolkata

Prof. N. Ravishankar, Materials Research Centre, Indian Institute of Science

Prof. G.U. Kulkarni, Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore

Prof. Vijay B. Shenoy, Materials Research Centre, Indian Institute of Science

Appendix B

Education and Research at the Atomic Level for Nanotechnology*

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In order to work with materials at the nanoscale, an ability to identify what is actually there and how it is held in place along with a sense of what this does for the properties of the structure seems an indispensable facility that one must have. The approach does, of course, depend somewhat on what actually is the property, structure and material that is the target of the preparation but sometime, somewhere one needs to know what is actually there. Otherwise (and perhaps too often) we rely on guesswork with theories built on the slimmest of clues as to what is happening. In this talk, I will address the approach of scanning transmission electron microscopy with particular reference to annular dark field imaging (ADF) and electron energy loss spectroscopy (EELS) as an emerging technique for what I like to describe as 'materials pathology', i.e., the science of learning what is actually there rather than what we thought we had put there as well as the clues that we can learn about what this has done for the properties. I will illustrate the approach with examples drawn from quantum well studies (GaN in AlN), growth of quantum rods of CdSe and efforts to place coatings of ZnS on CdSe to enhance the fluorescence efficiency of the dots. The improvement in equipment and techniques resulting from solving the aberration correction problem will be reviewed and the prospects of substantially improved performance identified. The education of scientists able to carry out this work will be reviewed, problems identified and solutions proposed.

* This talk is based on work supported over the years by the National Science Foundation and the New York State Science, Technology and Research Foundation (NYSTAR) through the Center for Nanoscale Systems at Cornell and the Department of Energy. My appreciation to D.A. Muller, Earl Kirkland, Todd Krauss and other collaborators for insights over the years and to K.A. Mkhoyan, Sara Maccagnano and Zhiheng Yu for examples drawn from current work in the group.

Nanowires, Nano interfaces and Nano Core-Shell Structures

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The author summarizes three aspects of work carried out in his laboratory on nanostructured materials during the last two years. Silver nanowires of diameter ~ 1 nm were grown within the channels of fluorphlogopite mica precipitated within a glass. By breaking up the continuous metal filaments very high dielectric permittivity was obtained for the nanocomposites. This was explained on the basis of Gor Kov - Eliashberg anomaly. Cadmium sulfide nanowires were also synthesized within the channels of Na-4 mica having a diameter of ~ 1.2 nm. Arrays of metal nanoparticles having a distribution of diameters were grown within a suitably chosen oxide glasscomposition. The nanocomposite exhibited a diode - like voltage - current characteristic. This arose because of the existence of interfaces of large and small metal particles - the latter behaving like a semiconductor. Silver and copper nanolayers were grown on the corresponding oxide particles respectively the latter having diameters of few nanometres. Detailed analysis of the optical absorption spectra of these composite species showed a metal to non metal transition in the nanoshells with diameters below a critical value viz., 2 nm. The interfacial phase created within a nanocomposite having a copper core - copper oxide nano core-shell structure was shown to behave like an amorphous phase. Lastly, the author discusses the educational background needed for young researchers to pursue this line of investigation.

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Flow Induced Generation Of Voltage in Carbon Nanotubes

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Our recent experiments (1) have shown that voltage/current is induced in single walled carbon nanotubes by the flow of water and other liquids. The induced voltage depends logarithmically on the flow velocity. The magnitude of the voltage depended sensitively on the ionic conductivity and on the polar nature of the liquid. This suggests that the dominant mechanism responsible for this highly sub-linear response involves a direct forcing of the free charge carriers in the nanotubes by the fluctuating Coulombic field of the liquid flowing past the nanotubes. Most interestingly, the direction of the induced current with respect to the flow direction can be controlled by the nature of the liquid and by voltage gating the nanotubes (2). In these experiments, the nanotubes are biased with respect to another reference electrode, thereby controlling the ions brought near the nanotubes. A general semi-phenomenological model will be presented involving dissipative coupling of charge carriers in the nanotubes to the fluidic Coulomb fluctuations with their correlations made spatially asymmetric by the flow. Recent applications using the flow-induced voltage generations will be discussed. We shall also present our recent results on the gas-flow induced electrical signals [3].

I thank S. Ghosh and N. Kumar for collaboration. It is a pleasure to thank Prof. C.N.R. Rao for the fruitful interactions and for providing the nanotube samples.

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Towards Symbiosis of Materials, Biology and Engineering: Emerging Nanostructures and Devices for Bio-Chem Sensing, Diagnostics and Therapeutics

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Recent years have witnessed a remarkable convergence of physical sciences, biology and engineering under the broad umbrella of nanoscience and nanotechnology. Indeed, there is an obvious synergy among these apparently disparate disciplines when the length scales of phenomena and structures approach the nanoscale. The emerging efforts in harnessing the connectivity of the nano-length-scales and the cross-disciplinary "nano-bio paradigm" promise considerable excitement for scientists and engineers, and tangible prospects for revolutionary applications for technologists as well as clinical practitioners. While intricate, precise and integrated systems approaches for complex bio-nano-structures with nanoscale precision and accuracy are still evolving, sufficient progress has been made to demonstrate proof-of-concept devices or applications based on functional nanostructures.

Our efforts in these areas at Northwestern are focused on not only advancing research at the interface of physical/life sciences and engineering, but also to develop integrated curricula and educational opportunities to mentor and train new generation of scientists and engineers with the common platform of complex hierarchy of length-scales and intricate architecture - across physical, life sciences and engineering.

The presentation will focus on two interrelated aspects of bio-nano structures: (a) novel bio-chem sensing and diagnostics, (b) site- and target-specific therapeutics. Embedded in these scientific themes are specific advances in:

- New nanopatterning approaches for functional soft, hard and hybrid nanostructures, which are prerequisites for patterning sensor arrays,
- Novel signal transduction and detection mechanisms in micro/nano-cantilever-based sensing and diagnostics, particularly related to remotely addressable embedded piezo-MOSFETs, and
- Synthesis, characterization and applications of magnetic nanostructures for therapeutics, such as targeted drug, biochemical and gene delivery.

It will be argued that emerging nanoscience and nanotechnology go beyond the "hype", and present realistic opportunities for creating a symbiotic ambiance for physical and life science - integrated on an engineering platform.

Molecular Tailoring of Monolayer Protected Nanoparticles

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We have been involved in the preparation and characterization of noble-metal colloids with specific applications in biology and chemistry. We aim to utilize our expertise in organic synthesis toward the designing novel compounds with desired functionalities that can then be employed as capping agents in preparation of noble-metal colloids (nanoparticles) endowed with capability of biological/ chemical applications. For example, we have found that gold colloids coated with hydrophilic and hydrophobic cationic lipid-analogues showed contrasting interactions with model lipid membranes.

Interfacing Nanomaterials with Biology

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The study of the synthesis, exotic properties, assembly and potential commercial application of nanomaterials is an extremely important topic of research in the area of advanced materials. While inorganic nanomaterials are expected to play an important role in the semiconductor and composites industries, a relatively new area of research is emerging at the interface between inorganic nanomaterials and biologicals such as amino acids, proteins, DNA and whole cells with exciting application potential in biosensing and pharmaceutical industries. During the course of this talk, I will cover some of the recent developments in this fascinating area from my lab in Pune. I will describe our efforts aimed at synthesizing water-dispersible gold nanoparticles capped with amino acids [1]; immobilization of enzymes on polymer microsphere-tethered gold nanoparticles [2] and the emerging area of nanobiosynthesis of inorganic materials using microbes and extracts of plants [3-5]. The work is highly interdisciplinary and I will describe my personal experiences in attempting to make things work/happen.

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Self Assembled Opal and Inverse Opals as Photonic Band Gap Structures with Waveguide Defect

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Self assembled colloidal structures provide a simple and effective fabrication method for photonic band gap (PBG) structures, without the need for expensive fabrication facilities. The self assembly of colloidal spheres results in the face centered cubic or the hexagonal close packed opals, and these do not have a photonic band stop regions, only pseudo stop regions, because a small gap only exists in one direction [1]. The alternative, the inverse opal, obtained by filling the spaces between the spheres with a suitable material, and then extracting the spheres to leave air holes, does have a band gap or band stop region, where electromagnetic waves in a particular frequency range are reflected. The index contrast ratio between the hole material, usually air, and the fill material needs to be at least 2.8 for this stop band to occur [2]. Introducing defects in these photonic band gap materials allows for localized trapping of the electromagnetic wave, and at the stop bandfrequencies should result in extremely high Q cavities. To take advantage of this, it also becomes necessary to have some channel of communication with this high Q cavity. However, placing a well defined defect in colloidal opal or inverse opal is difficult, and in this paper, a defect in the form of an optical waveguide is proposed. Thus, a cavity may be formed as desired, and the guide provides a means of connecting this cavity to the outside world. Thus, the project involves burying an optical waveguide in a colloidal opal as a first step, and subsequently in an inverse opal, and in this paper this first step of the project is discussed. A silicon nitride waveguide was first fabricated, with a rib of silica. Si_3N_4 was grown on a silicon substrate, which had previously a 6 μm of thermally grown SiO_2 layer. The nitride and silica are patterned to have a nitride guide supported by the rib of silica. The waveguides were characterized for propagation loss using the cutback method. Silica spheres of 710 nm diameter were fabricated using the standard Stober method [3], modified to ensure that the distribution of sphere size was less than 2%, and that an extremely low fraction, less than 0.3% of the spheres had aggregations or adhesions. The waveguide was coated by the spheres to form the opal using the meniscus process [4], modified to uniformly coat wafers 3 cm × 1 cm in size with nonplanar surface. The effect of coating on the waveguides has been characterized.

The paper will discuss the results of simulations of the waveguide and the opal, the former using a beam propagation code, and the latter using a FDTD code. The experiments to obtain the silica spheres will be discussed, together with the coating method. The future work which includes the coating of the waveguide without the rib, and to use this as the template for the inverse opal, 1 will also be discussed.

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Transition metal-doped semiconducting nanocrystals:

Tuning and understanding the optical properties

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Doped semiconductor nanocrystals form an important class of materials from the technological point of view.[i] They are mainly interesting because of two reasons. Doped semiconductor nanocrystals exhibit sharp and high intensity luminescence[ii] and thus, are potential candidates for applications in light emitting devices and displays. By doping various metal ions such as Cu^{2+}, Eu^{3+} and Mn^{2+}, it has been possible to obtain luminescence in the blue, green and orange regions of the visible spectrum.[iii] Mn-doped ZnS and Mn-doped CdS nanocrystals exhibit high luminescence quantum efficiencies. It is also possible to tune the luminescence wavelength by using a different host semiconductor. For example, Mn^{2+} in ZnO emits[iv] at a much shorter wavelength compared to Mn^{2+} doped into either ZnS or CdS. Another aspect of doped semiconductor nanoscience is the possibility of obtaining magnetism in such systems. For example, it has been predicted that Mn^{2+} doped GaAs, which is a known half-metallic ferromagnet in the bulk, can possibly retain the magnetic properties down to very low sizes,[v] thus, making it possible to design “spintronic” devices in such small size regimes.

In this talk, I shall discuss several of these issues based on our recent results in the area of transition metal (primarily Mn) doped semiconducting nanocrystals with sizes in the quantum confinement regime.

The results presented are based on collaborative work carried out with A. Anand, S.V. Bhat, B.N. Dev, N.A. Hill, J. Nanda, S. Sanvito, B. Satpati, P.V. Satyam, and S. Sen Gupta.

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Non-Volatile Silicon Memories at the Nano-Scale: An example straddling materials science, semiconductor physics, and large-scale integration architecture

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The key challenges for memories that operate at the nanoscale, and are compatible with mainstream nanoscale CMOS, are in achieving the performance characteristics that make integration of 100's of millions or more of such devices useful together with the reproducibility necessary for manufacturing. Use of single or few electrons by utilizing the reduced dimensions, i.e. smaller number of states and larger charging energies, is very appealing as a concept, but needs to address the increased variance, smaller signal, and numerous other consequences of reduced collective phenomena. Inorganic media, such as silicon, do have the underlying desirable characteristics of manipulation of energy barriers and control, e.g. thin oxides provide high barrier heights and close electrostatic control, and the ability to have reasonable currents, necessary for fast sensing, due to the larger state density and velocity in bands. Coupling few electrons to a transistor channel provides a structure with power gain and the necessary current for fast memory-state detection as well as compatibility with CMOS. Several key ideas of recent times, from the use of nanocrystals, use of defects, and decoupling of storage from read process, provide paths where power, speed, technology compatibility, and variability is addressed. We discuss several of these approaches and their attributes focusing on the underlying interdisciplinary science and engineering issues, and conclude with the implications for education.

Bio-MS for Cardiac Diagnostics

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In this talk, we will look at the current status of an ongoing effort in The Electrical Engineering department at IIT Bombay on the development of an integrated system to provide point-of-care diagnostic support for cardiovascular diseases. The system under development monitors the molecular markers to detect cardiac attacks, especially incipient cardiac attacks that go undetected before major/fatal attacks occur. The system comprises of "infarcSens" or "iSens", which is a cantilever & molecular FET based affinity biosensor array for sensing myocardial infarction & subsequent cardiac status prognosis, using a suite of molecular markers. The sensing electronics and the associated data management software, for tracking the markers with time required for creating an epidemiological database, is also currently being developed. A multidisciplinary team from the departments of Elecrtrical, Bioengineering, Chemistry, Material Science and Mechanical Engineering is currently working on this project, which is supported under the NPSM programme by the Govt of India.

As part of this presentation, we will also discuss some of the other interdsciplinary research activities involving the speaker, and highlight the issues with interdisciplinary research and educational training.

Nano-technology and the 'post CMOS' world

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After four decades of unprecedented exponential growth silicon CMOS is approaching its limits. This offers both challenges and opportunities for the technological community since radical new structures and deeper understanding of the transport physics are required. The extremely aggressive structures targeted by the 'end' of the silicon roadmap raise the bar for the introduction of any new nano-technology and almost certainly mean that this technology will be forced to co-exist with CMOS on the same chip. This talk will discuss silicon CMOS options for the future and the requirements for the new nano-technologies highlighting research being done at industrial labs such as IBM to meet the future challenges.

Ge Based High Performance Nanoscale MOSFETs and Integrated Optical Interconnects

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It is believed that the difficulty in scaling the conventional Si MOSFET makes it prudent to search for alternative device structures, new material and fabrication technology solutions that are generally compatible with current and forecasted installed Si manufacturing. The saturation of Si MOSFET drain current upon dimension shrinkage limits the prospect of future scaling. Historically it has been believed that as the device dimensions are scaled down the high field carrier velocity saturation diminishes the difference in performance of MOSFETs in different materials. However, it has been recently pointed out that a fundamental scaling limit for MOSFETs is the source injection velocity into the channel limiting the drain current. The lower effective mass (and lower valley degeneracy) of Ge could alleviate the problem by providing a higher source injection velocity, which translates into higher drive current and smaller gate delay.

Scaling of VLSI circuits can pose significant problems for interconnects, especially for those responsible for long distance communication on a high performance chip. The near-infrared photodetection and compatibility with Si technology of Ge-based materials, allow simultaneous fabrication of photodetectors and Si CMOS receiver circuits in a monolithically integrated fashion. Such technology could be used for on-chip optical interconnections in global signaling and clocking.

Surface passivation for gate dielectric and field isolation and n-type dopant incorporation are the two classic problems that obstruct CMOS device realization in Ge. In this paper we present a review of the recent activity in this area and application to MOSFETs and photodetectors. High mobility MOSFETs have been demonstrated in bulk Ge and in nanowires with high-k gate dielectrics and metal gates. In order to enhance performance and continue scaling MOSFETs to the sub-20nm regime, novel, high-mobility materials like strained-Si and Ge (or SixGe1-x) are actively being researched for incorporation into the channel. We have developed undoped, Center Channel (CC) NMOS and PMOS FETs that incorporate novel transport principles, which fully exploit the advantage of high mobility materials. High performance Metal-Ge-metal photodetectors with asymmetric workfunction electrodes to suppress IDARK have been demonstrated for optical interconnect applications.

Submicron InP Bipolar Transistors:Scaling Laws, Technology Roadmaps, Fabrication Processes, & High Frequency Circuits

Mark Rodwell,
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Despite the superior integration scales of CMOS, bipolar transistor integrated circuits find applications in 10-40 Gb/s optical transmission, in microwave transmitters and receivers, and in high-frequency mixed-signal ICs . While Silicon Germanium heterojunction bipolar transistors dominate over InP in commercial applications, Indium Phosphide HBTs compete for the highest-frequency applications, particularly ADCs & DACs for radar.

As compared to SiGe devices, InP HBTs offer larger collector electron velocities, smaller base sheet resistance, and larger (breakdown x ft) products. In contrast, SiGe processes are much more highly scaled in both junction dimensions and in current density and employ processes providing much better extrinsic parasitic reduction. Digital circuit speed is therefore comparable in the two technologies. SiGe HBT processes are more nearly planar than InP, and submicron emitters are formed not by semiconductor etching but by semiconductor regrowth. For these reasons SiGe HBT processes exhibit much higher yield (hence lower IC cost) than InP in the high-volume fabrication of large ICs, although InP is cheaper in lower-volume production due to the simpler fabrication facilities required. The talk describe efforts at UCSB to develop highly scaled InP HBTs. Device performance must first be analyzed in terms of parasitic elements, small-signal figures-of-merit, and --much more importantly-- in terms of performance in broadband circuits and in logic. Implications in terms present and emerging HBT designs will be discussed, including the role of current density, collector capacitance reduction, transit times, and emitter and base resistances. Scaling laws will be introduced, and several advanced submicron fabrication processes described.

Our best InP HBTs today have ~370 GHz f_τ and ~460 GHz $f_{\max}$, and are suitable for ICs beyond 200 GHz. I will describe our demonstration 50-200 GHz IC designs. Small-signal RF ICs include single-transistor HBT amplifiers exhibiting 6.3 dB gain at 175 GHz, and three-stage amplifiers having 8.5 dB gain at 195 GHz. InP DHBT power amplifiers include a 75 GHz, 80 mW design and -very recently- a 172 GHz single-stage power amplifier producing 7.5 mW with 5.0 dB associated gain, and a 148 GHz two-stage power amplifier producing 14.5 mW with 4.6 dB associated gain. Digital IC results include (a standard benchmark) static frequency dividers operating at 152 GHz

Mark Rodwell (Ph.D. Stanford University 1988) is Professor and Director of the Compound Semiconductor Research Laboratories and the NSF Nanofabrication Infrastructure Network (NNIN) at the University of California, Santa Barbara. He received the 1997 IEEE Microwave Prize and was elected IEEE Fellow in 2003.

NANOCRYSTALLINE THIN FILMS: A BRIDGE BETWEEN NANOSCIENCE AND NANOTECHNOLOGY

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While there is still a lot of basic science interest in investigating finite size effects in various classes of solids such as metals, semiconductors, superconductors, magnetic and ferroelectric materials, research in each of these areas is driven by exciting current and futuristic applications. Most of the early applications, such as in catalysis, were in nanocrystalline powders. Bulk nanostructured materials and alloys have also been investigated from the point of magnetic and mechanical properties. However, it appears very clear that for most of the high-end applications in optoelectronics, non-linear optics and so on, it is essential to synthesize nanocrystalline thin films (NCTF) with well controlled grain sizes on suitable substrates. We discuss the importance of NCTF in nanotechnology research with specific examples from different classes of nanomaterials

Mechanical Response of small volumes of material

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Depositing a very thin film of material on a surface has been found to be an amazingly efficient method of providing protection to mechanical, biological and electronic systems of length scales many orders greater than that of the film thickness. Form soft condensed matter at nanometric molecular thinness to super hard ceramics of micrometric dimensions have found use to protect mechanical machineries such as engines, gears, bearings and other components which transmit power. While protection is sought from chronic to catastrophic damage, chemical attack and erosion these microscopic films are required to ensure smooth power transmission at a minimum level of dissipation. While these practices have evolved empirically over a period of time interest has grown exponentially over the last decade to understand the mechanical response of these films with a view to optimize the materials, component geometry and processing routes to meet enhanced conditions in which these machineries are required to operate. As such engineering solutions have become extensive, the knowledge has crossed the barrier of research and has entered designers compendia and encyclopedia. An engineer of tomorrow has to be as familiar with the solutions derived from disparate areas of mechanics, material science, physics, physical and organic chemistry. Thin film technology which synergises principles from these disparate areas into an interdisciplinary envelope hammers the doors of our undergraduate and post graduate curricula. In this talk I shall focus on two examples of thin film nanotribology.

Automobile manufacturers have dreamt to mass manufacture light weight automobile engines. Of the many problems which remain in realizing this dream a major one is how does one protect a light weight cylinder liner in actual operation. We have worked on design of organic molecules which can be grafted on aluminium as a monomolecular layer to support large normal and tangential loads met in an engine bore under conditions of thermal cycling. Here we will briefly talk about the approach and methods we adopt to determine stiffness, damping, adhesion and friction of such molecules to demonstrate that the nanometer scale properties have a large bearing on the actual operational efficiency of the engine.

The second example I cite is that of hard ceramic films of micrometric dimensions used to provide protection to gears and cutting tools to enhance the durability of a cheap substrate by many orders. Our work on nanoindentation of columnar titanium nitride films of 1 to 5 microns thickness deposited on steels has led us to an understanding of how such films are damaged in practice. A synergy of nanomechanics, x-ray diffraction studies and detailed electron microscopy has shown us that there is an optimum thickness for such films for a given substrate plasticity; where for an application such as coating of a hard tool tip chronic damage is delayed by depositing a thick film while the protection from an environmental chemical attack of a soft metal is best served by a very thin film.

Static Non-contact and Transient Signal Atomic Force Microscopy

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Iowa State University

In this talk two new methods of investigating matter at the nano-scale will be presented: Static Thermal Noise Based Atomic Force Microscopy (AFM) and Transient Signal based AFM. Using the equivalent resonant frequency of the micro-cantilever as a measure of the tip-sample separation and the detection of the resonant frequency from the thermal noise response of the cantilever, the tip can be maintained at nanometer separation from the sample for extended periods of time. It will be shown that with this method, topographic oscillations in the sub-Angstrom range are detectable. In the Transient Signal based imaging, by utilizing the cantilever model the fundamental limitation on the bandwidth imposed by the high quality factor is alleviated. For detection related imaging, such systems based approach provides orders of increase in bandwidth. The relevant interdisciplinary research and teaching issues will be highlighted.

Charge Storage Redox-Active Molecules for Hybrid Silicon Molecular Memories

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The field of molecular electronics is gaining interest due to the miniature size of molecules, which may enable memory and logic applications in the nano-scale. Particularly attractive is the hybrid silicon/molecular approach because of its unique nature of combining the molecular electronic elements with existing silicon technology. This approach can also provide a bridge between CMOS-only and future molecular-only technologies. The advantages of molecular-based memory devices include nanoscale size, low voltage operation and multiple-state properties. In this work, redox-active charge-storage molecules are incorporated into silicon structures to generate a class of nano-scale molecular electronic devices.. Application of an oxidizing voltage on these molecules, which exhibit charge states at distinct voltages, causes them to lose electrons and acquire a positive charge (write state). Electrons are transferred back to the molecules from the substrate when a reducing voltage is applied (erase state). In this presentation, the properties of SAMs of redox-active molecules on very thin SiO_2 layers will be discussed. The redox potentials, tunneling probability and retention times can be tuned by varying the size of the linker and the oxide thickness. The properties of these monolayers and their dependence on oxide thickness, measurement frequency and amplitude will be discussed. Next, the role of substrate engineering to enhance the properties of molecules will be presented. The use of N+ (or P+) pockets embedded in p-well (or n-well) Si substrates as a means of obtaining multiple states from a two-state molecule will be discussed. We will also report on utilizing N+/P and P+/N diodes to increase the charge-retention times of redox-active monolayers. Both of these strategies illustrate engineering of the silicon component in hybrid silicon-molecular devices. We believe that co-engineering both the silicon and molecular components will enable access to novel device functionalities that may not be possible with silicon or molecular devices alone.

Probing nanometer scale dynamics of molecular & cellular assembly using an optical tweezer

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Biomolecules & Cells self-assemble to form long-range dynamic order. In this talk, I will describe experiments, using an optical tweezer, to study the spatio- temporal correlations & dynamics of such ordered structures. In particular experiments related to the measurement of correlated dynamics of self-propelled particles and the dynamics of membrane nanotubulation will be presented. Our results may also have applications in the development of nanowires and nanofluidic devices.

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Electrical properties of confined organic structures

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We shall discuss results of our recent studies on electrical transport properties of ultra-thin multilayer metal-organic films grown by Langmuir-Blodgett **(**LB) deposition techniques. We have also observed one-dimensional ratchet potential in nanowires of a conducting polymer formed in nanopores through a controlled polymerization process.

We have developed a bilayer film of Au nanocluster on gadolinium stearate. These films behave like a nanostructured network of islands and interconnects that exhibit non-ohmic I-V characteristics when measured laterally across the film using a conducting AFM tip. The morphology and electrical properties of the Au nanoparticle layer changes remarkably depending on the surface pressure of the Langmuir monolayer employed for its transfer on to the gadolinium stearate layer.

The resistance of the nanowires of conducting polymer can differ by several kilo ohms as the direction of current flow along the length is reversed. The directional resistance becomes more pronounced with decrease of diameter of the nanowires and this result opens up a possibility of fabrication of charging rectifier in nanowires of conducting polymer. We could explain this ratchet effect, which reduces with reduction of temperature, using phonon activated hopping theories by invoking growing extent of delocalization along the nanowires.

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Soft routes for alternate lithography

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Optical and e-beam lithography have been used to create features of size few tens of nanometers. Most of this lithography are based on or evolve from the CMOS technology. This is a viable route for producing ULSI with sub 0.1µm. resolution. There is, however, need for alternate routes to produce nano structures. that can be integrated at some stage to the CMOS technology. These routes are based on wet chemistry based soft lithography routes. Advantages of these routes are that they can be used to produce functional materials often in the form of an array, which have the potential to function as device or part of a device. An interesting question that would need an answer whether some of these alternate lithography can be integrated in present from or with some modification to the standard CMOS based nanotechnology. While the answer is not obvious it can be appreciated that such an integration can lead to immense progress in this field.

The alternate routes are : nano imprinting, solution and sol-gel based growth in templates such as porous anodic alumina, growth in templates formed in block co-polymers, growth on patterned seeded surface, pulsed local oxidation by conducting AFM and dip pen lithography (DPN). In my talk I will mention briefly these techniques.

The general presentation will be followed by specific results that have been obtained by us using three alternate routes. By using template based growth we can produce an array or individual nanowires of metals and functional oxides. Functional oxide dots and nanowires have been made on Si substrate by using dip pen lithography. We have also used seeded growth technique to create arrays of nanowires of ZnO on Si. My presentation will involve a brief description of these specific results and I will discus the advantages of these specific routes and the advantages that may be achieved by integrating them with CMOS routes.

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Metal Nanoparticles : Synthesis, Assembly and Melting Behaviour

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The talk will focus on our research on metal nanoparticles. The first part will focus on the synthesis of metal and alloy nanoparticles by reduction of metal salts using chemical means. Some of the fundamental mechanisms relating to the formation of nanosized crystals will be highlighted. In the second part, a new method to produce ordered arrays of metal nanoparticles on reconstructed surfaces will be presented. This method relies on a highly site-specific heterogeneous nucleation of liquid metal from the vapour phase. The third part will focus on the melting behaviour of embedded metal/alloy nanoparticles in a metal matrix.

Electrical properties of ultrathin nanocrystalline gold films formed at the organic-aqueous interface

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Liquid-liquid interfaces offer the requisite conditions for the preparation of ultrathin nanocrystalline metal and semiconductor films. We have developed an elegant one-step synthesis of nanocrystal arrays at the organic-aqueous interface wherein an organometallic compound dissolved in an organic layer reacts at the interface with the reducing agent present in the aqueous layer. The material formed at the interface corresponds to an ultrathin nanocrystalline film consisting of closely packed nanocrystals coated with the organic species present at the interface. The novelty of this method is that it involves a finite growth rate of the ultrathin nanocrystalline film with controllable parameters such as temperature and concentration. In addition, the method yields free-standing films which can be used for further investigations.

In this talk, the properties of nanocrystalline films consisting of closely packed Au nanocrystals will be presented. The size of the nanocrystals constituting the film markedly increases with temperature, but the concentration of the organometallic precursor has little effect. The nanocrystals in the film are separated by ~ 1nm due to the organic coating. The films are generally smooth and continuous over a length scale of several microns, the thickness being in the range of 40-140 nm. Electrical resistance measurements using the four-probe method show that the film prepared at room temperature was semiconducting with a high resistance (~ few mΩ). The resistance gradually decreases with increase in the reaction temperature, yielding metallic films beyond 60ºC. UV-Vis absorption spectra reveal that the surface plasmon band of gold is red-shifted markedly in the films due to dipolar coupling between particles, the magnitude of shift reflecting the state of aggregation of the nanocrystals in the films, paralleling the changes in the electrical resistance. Interaction with alkanethiols markedly perturbs the films separating the nanocrystals, the magnitude of the perturbatin depending on the chain length of the thiol. Such perturbation also affects the electrical properties of the films, the long chain thiols increasing the resistance. However upon interaction with a conjugated molecule, the resistance of the film drops.

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Nanophotonics: the manipulation of light in nanostructured materials

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The field of photonics has generally been concerned with the generation, detection, guidance, and manipulation of light. This has invariably involved the manipulation of the two fundamental particles of modern information technology: the electron and the photon. Nanophotonics is the confluence of activities in photonics and activities in the fabrication of materials structured at the optical sub-wavelength scale. The light-matter interactions in this case are deliberately designed to lead to interesting and useful phenomena. For most materials of interest, sub-wavelength scale structuring is equivalent to having materials with artificial physical features (with spatial index or band gap contrasts) that are on the order of tens to hundreds of nanometers. The interaction of the light field with such features leads to a number of interesting and useful properties for manipulating light. There are primarily two major classes of interactions: (1) an interaction where light is generated or absorbed, or (2) an interaction where it is confined (or excluded), or guided (or not guided). In the first case, one is primarily interested in materials that can generate light—these are usually direct band gap semiconductors. Here, the relevant nanostructures are the so-called quantum dots; they are direct, low band-gap semiconductor nanoparticles surrounded by large band gap outer materials. The spatial extent of a quantum dot is on the order of a *de Broglie* wavelength of an electron in the particular semiconductors constituting the dot. One of the unique features of quantum dots is the emergence of a new energy bandstructure that can be used in the design of novel light sources and detectors. To date, useful quantum dots have been fabricated by self-assembly techniques. Both epitaxial and colloidal quantum dots have been demonstrated. The second interesting mode in which light interacts with a nanostructured material depends critically on the contrast of the index of refraction in the material. This index contrast, and its particular pattern of variation in a two-dimensional or three-dimensional bulk material, can lead to guidance, confinement, or exclusion of photons in or from extremely small volumes. Materials structured to control light in this fashion are called photonic (band gap) crystals. There is an analogy between semiconductor crystals and photonics crystals. The analogy exists because photonic crystals typically have periodic two- or three-dimensional index contrasts that can lead to forbidden frequency (wavelength) gaps that are analogous to the energy band gaps of semiconductors.

This presentation will discuss the underlying concepts and opportunities in nanoscale structured materials for photonics. In particular, we will discuss the use of quantum dots in the design of a new generation of light sources and detectors. We will also discuss the potential to incorporate quantum dots in photonic crystals for the design of truly integrated nanophotonic circuits. The vision of integrated nanophotonic circuits is fraught with challenges; some of these will be discussed.

Molecular and Mesoscale Modeling and Simulation in Nanotechnology: Research and Education

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Molecular and larger length-scale modeling and simulation are playing an increasingly important role in fundamental understanding of nanoscale phenomena and as well as in technological applications. Detailed information available from molecular simulations provides excellent opportunities for education and outreach when combined with with visualization tools. I will briefly present examples from my group's research that focus on (i) understanding biological structure and function in non-biological contexts (e.g., protein under high pressures, enzymes in non-aqueous media) , and (ii) multiscale modeling of polymers. We have recently developed "Molecularium" – an education and outreach effort in which molecular level concepts are taught to general public through development of animation movies that are projected in a planetarium dome. I will present the progress of this project. Both research and education efforts are funded by the US National Science Foundation.

SIMULATIONS OF COMPLEX SYSTEMS ACROSS SCALES: CONNECTING THE NANO TO THE MACRO WORLD

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The current fascination with nanoscale systems for scientific and technological applications focuses mostly on the properties of object with characteristic size of order nanometers. This study needs to be complemented by how such nanoscale features connect to macroscopic systems, which are their natural host environment. The connection of atomistic nanoscale structure to the macroscopic behavior of materials is an oen and challenging issue in computational materials science.

In this talk we will discuss the development of methodologies for simulations across disparate length scales with the aim of obtaining a detailed description of complex phenomena with examples ranging from fracture mechanics to biological motors. The methodologies are based on density functional theory approaches at the microscopic scale, on molecular dynamics simulations at the mesoscopic scale and on continuum approaches at the macroscopic scale. We describe the key ideas behind the links across the scales and how these are implemented in specific cases. The systems and phenomena we will consider as representative examples are: the nature of crack propagation in brittle solids like crystalline silicon, the role of defects and impurities in changing the ductility of metallic solids like aluminum, the role of external stress in the conductivity of DNA nanowires, and the functioning of biological rotary motors.

Pattern formation in soft thin films

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Pattern formation in thin films is of interest both from scientific and technical viewpoints especially since it provides for a route to produce patterns at the nanoscales. This talk will briefly survey the area of pattern formation. A particular example of patterning of soft films will be dealt with in detail. Outstanding problems will be discussed.