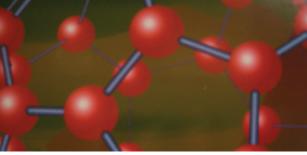
Stony Brook University Nanotechnology Research Projects











Nanotechnology Research Projects

The technology revolution is getting smaller...

Nanotechnology, science and engineering at the scale of individual atoms and molecules, gives new meaning to the idea that small is beautiful. The potential of nanoscale devices offers us a vision of miniaturized biomendical implants not only patrolling our arteries as an early warning system, but also delivering drugs as needed *in situ*; sensors detecting and reporting evidence of anything from toxic materials in shipping containers to changes in air quality to traffic delays; and the "smart" home, "smart" office building and "smart" city. But this is the end of the story. Getting there is an exciting journey, for another of the beauties of nanotechnology is that, without a single addition to the periodic table, familiar materials become things rich and strange. Gold, for example, is one of the more stable elements in nature, yet at the nanoscale it is one of the most active: small is also new. To realize the vast promise of nanotechnology, researchers must first understand the properties and behavior of these materials in order to develop the astonishing range of potential applications.

These studies require contributions from many disciplines to move the most quickly from basic research to commercialization. Stony Brook's strong programs in materials science, the engineering disciplines, physics and chemistry illuminate basic properties and fabricate and test engineered materials and new devices, the mathematical sciences and computer science model structure and behavior, and biomedicine, biomedical engineering, the life and marine sciences explore the significance of nanotechnology for living things. The results of these inquiries range across the broad spectrum of nanotechnology, from gene and DNA sequencing to applications for clean energy to tissue engineering. Stony Brook University researchers not only excel in pushing the technology frontier forward, but have built a cooperative industry network, where corporate researchers work side by side with university faculty and students to perfect potentially marketable new technologies. Nanoscale devices currently being developed at Stony Brook include hybrid CMOS-nanowire semiconductor chips able to deliver the same computing power at one-tenth the size (recently prototyped by HP researchers), implantable drug delivery systems and internal sensors tracking the condition of jet engines. These and the many other efforts described in this brochure, involve collaboration with Brookhaven National Laboratory and the private sector – regional, statewide, national and international. Guided by partnerships these projects address leading edge science and technology issues, culminating in the transfer of new technologies to commercial application, disseminating life-saving and life-improving technologies while creating new means for competitive advantage and new economic assets.

The projects and programs described here are a modest representation of the depth and breadth of Stony Brook's commitment to the research in the field of Nanotechnology, and we invite you to take a look.

Gail Habicht Vice President for Research Yacov Shamash Vice President for Economic Development and Dean, College of Engineering and Applied Sciences





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Nanotechnology at Stony Brook

BNL Center for Functional Nanomaterials

Emilio Mendez

The Center **Functional** for Nanomaterials (CFN) Brookhaven National Laboratory (BNL) represents a major resource for Stony Brook University's nanotechnology program. The CFN is a user-oriented research center that has its own scientific program and at the same time offers broad access to its state-of-the art facilities through a vigorous external users' program. As a premier user facility for conducting interdisciplinary nanoscience research, the CFN serves as a focal point and enabler of advanced materials study. Together with the National Synchrotron Light Source (NSLS), and, in the future, the NSLS-II, these facilities complement each other to enable the nanoscale revolution. The synergy among these world-class facilities, with Stony Brook and Brookhaven's scientific staff working collaboratively with university, industrial and government laboratory researchers, offers unique opportunities for breakthroughs in nanoscience and nanotechnology research.

The capabilities at the CFN available to staff/external users are arranged into seven major facilities:

- Materials synthesis: Chemical vapor deposition and other synthesis methods for the growth of nanowires and quantum dots; biofunctionalization of nanoobjects and surfaces
- 2) Nanofabrication: Nanopatterning via optical, electron-beam and nanoimprint lithography; wet or reactive-ion etching, focused ion-beam, thin-film deposition by evaporation and sputtering for materials processing and device fabrication in a class-100 facility
- Proximal probes: An array of scanning probe tunneling and atomic force microscopies for advanced surface and interface analysis
- 4) Electron microscopy: Most advanced transmission electron microscopy that, in addition to imaging, allows the study of electronic, magnetic and optical properties at the atomic level

- 5) Optical spectroscopy: CW and ultrafast spectroscopy tools for the study of optical processes, and their dynamics, in nanomaterials, down to single molecules
- 6) Dedicated beamline at the NSLS: Especially designed for small- and large-angle x-ray scattering and ideally suited for the study of soft materials and interfaces
- 7) Theory & computation: Staff and computational tools directed to understanding the formation and structure of nanoscale materials and associated electronic, optical and chemical phenomena

(DOE, NSF, NIH)



Ethics and Nanotechnology

Shmuel Einav

We are quickly approaching the technological ability to fabricate machines and devices that can manipulate items at the atomic level, as well as developing molecular based computers and robots and treating diseases at their inception. While it is not difficult to see the benefits of nanotechnology, many can observe the risks in developing creation power assemblages and components. We have begun to explore the health and environmental impacts Nanotechnology. Other ethical issues stem from increasing diagnostic power of cellular medicine. Eric Drexler, Nanotechnology best known visionary, claimed that the true power of Nanotechnology is in molecular manufacturing. We are looking into the potential danger of nanomaterials to health and the environment. We are on one hand encouraged by the ability of nanoparticles to cross the blood-brain barrier and thus benefit drug delivery to the brain, but on the other hand may present serious workplace dangers and the level of deployment.

We are investigating the convergence of nanotech, biotech, information technology and cognitive ability, on social issues, ethical behavior and privacy. We are planning to integrate ethical issues in our nanotech activities, and produce ethical guidelines. Our nanoethics activities are aimed in three different directions:

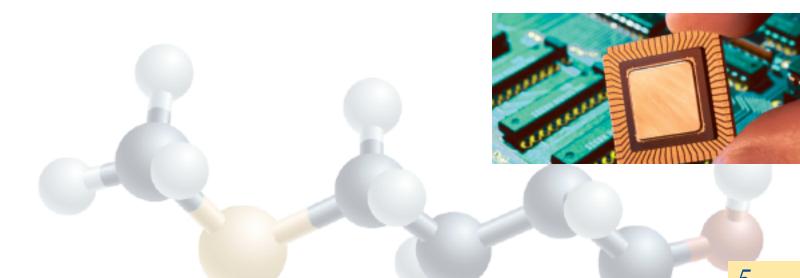
- a) awareness within research and development initiatives;
- b) devising opportunities for open and genuine discussions with members of the university community and the public and
- c) education in our graduate programs.

(CEAS)

New Atomic Force Microscope

Steve Smith

The Center of Structural Biology is developing, together with LifeAFM Inc., a new atomic force microscope that has significantly better resolution than the currently available. Several collaborative projects are in progress that demonstrates the capability of the instrument. As a result we expect that our technology will set the standard for atomic force microscope. The technology would be very appropriate for any initiative in nanoscience and nanotechnology, and strongly highlights a unique capability at Stony Brook. (NCRR)



Nanotechnology in Biology

High Throughput Ultra-sensitive Gene and DNA Sequencing

V.B. Gorfinkel

The main goal of the project is to bring our novel DNA sequencing instrument from the research stage via the development stage to the pilot project testing stage. The instrument development will be carried out at Stony Brook, and sequencing technology development will be carried out at our Health Science Center (HSC) and Cold Spring Harbor Laboratory. (NYSTAR, NIH)

Development of Biologically Active Nanocomposites Using Human Blood Coagulation Protein

Jolyon Jesty

The major goal of this exploratory study is to characterize interactions between blood coagulation proteins and nanomaterials. Bionanocomposites will be prepared comprised of a nanomaterial and a major element of the human clotting system. The initial focus will be on polymeric nanofibers prepared by electro spinning in the presence of either fibrinogen or platelet microparticles. Interactions between the nanoparticles and the blood will be at the molecular level through SEM, surface plasmon resonance, and atomic force microscope. (NIH)

Gene Regulation and Biological Pattern Formation

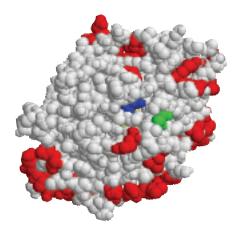
John Reinitz

We are engaged in a long term project to characterize the dynamics (physiology) of the segment determination process and control of transcription in the fruit fly {Drosophila melanogaster} means of an integrated approach that utilizes experiment, computation, and mathematics. The major goal of our work is to achieve an integrative understanding of the segment determination process as an emergent property of a network of genes, a copy of which is present in each of many cells. We are also engaged in making models of transcriptional control which are designed to predict the physiological action and expression patterns of modular enhancers from knowledge of their constituent binding sites. Both problems are being approached using an approach called "Gene Circuits".

The Gene Circuit method has four parts:

- 1) Construct a theoretical model,
- 2) obtain gene expression data,
- 3) fit the model to the data by large scale numerical optimization, and
- 4) learn new biology from the model. In addition to shedding new light on fundamental biological problems, we have developed new algorithms in support of points 2 and 3 above.

With respect to expression data, these include new methods of image segmentation, registration, classification, and background removal. These data have been placed on the web in a modern bioinformatics database. With respect to large scale optimization, we have developed both a new parallel simulated annealing algorithm as well a new Lagrangian Optimal Steepest Descent optimizer. (NIH)



Nanostructured Materials for Single Molecule Enzymology: A Field Trap Apparatus

Stuart McLaughlin

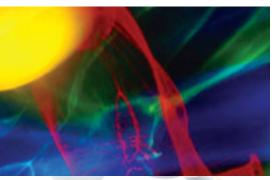
The long-term objective is to develop technology and instrumentation for measuring the activity of single enzyme molecules that change the charge of their membrane-bound substrates, e.g. lipases, kinases phosphatases. Combining microelectrophoresis and laser trap technologies, the field/trap apparatus uses the principle of the Millikan oil drop experiment: a silica bead coated with phospholipid bilayer replaces the oil drop and tightly focused laser beam replaces gravity. When an AC field is applied to the coated bead in a salt solution, the electrophoretic force displaces it from its equilibrium position in the laser trap. The displacement, measured with a fast quadrant diode is a proportional to the number of charged lipids (e.g. phosphatidylinositol. 4.5-biphosphate, IPI2) on the outer leaflet of the bead. When a solution containing enzyme (e.g. phospholipase C, PLC) flows past the bead, the proteins adsorb to the surface and change the charge on the bead (e.g. hydrolyze trivalent PIP2 form the neutral lipid diacylglycerol).

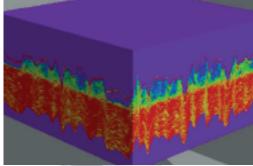
A prototype apparatus has been constructed to demonstrate proofof- principle and used to study PLC-delta. Specific aim 1 is to construct a new apparatus at Stony Brook that will be capable of detecting hydrolysis of 10-100 PIP2 by a single PLC on a bead, initially containing 10,000 PIP2, with a time resolution of 0.1-1.0 sec. Specific Aim 2 is to expand the field/trap approach by adding fluorescence correlation spectroscopy (fcs) capability, which will enable simultaneous measurement of the fluorescence signal from a single enzyme and its activity. The field/trap approach will be applied to study enzymes of great biological and medical importance: PLCbeta isoforms that produce two second messengers when activated by G proteins; the lipid kinase PI3K, which produces another class of second messengers that have been implicated in cancer; and PTEN, a lipid phosphatase that is a highly mutated clinically important tumor suppressor. (NIH)

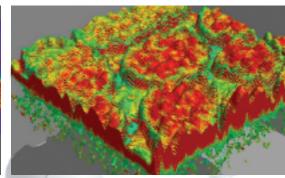
Modeling of Bio-molecules

Yuefan Deng and James Glimm

The central problem for molecular dynamics (MD) simulations of protein structure is the disparity between time scales for atomic vibrations and those for conformational changes. Typical time scales for conformational changes are not known, but have been estimated as of the order of a micro sec. The time step in an MD all atom simulation is of the order of a femtosec. so that that billions of time steps may be needed. This simple fact illustrates the central difficulty in the direct all atom simulation of structural biology. We have developed new tools applicable to a special purpose computer to be located at BNL, which allow the all atom simulation of molecular dynamics for a greatly extended time period, up to 10 micro sec. This algorithm will allow exploration of new regimes of biology in the binding of proteins, and their biological functions. (BNL)







Site-Specific Gene Therapy for Myyocardial Angioensis

Weiliam Chen

The research and development of genetic delivery for treatment of ischemic heart disease is the focus of many investigations. However current techniques of gene delivery are inefficient and very limited in scope. The objective of the proposed studies is to develop a biodegradable polymer-based DNA delivery system for sustained release of vascular endothelial growth factor (VEGF) to promote revascularization in ischemic myocardium. Specifically, the applicant proposes to: encapsulate DNA in small nanometer diameter particles with a poly-lactic-polyglycolic acid co-polymer, assess the in vitro delivery mechanism of nanoparticles using beta -galactosidase as a model reporter gene. and then finally to evaluate the efficacy of VEGF gene transfer in a rat cardiac injection model. These experiments may help establish the feasibility of using this delivery system for gene therapy. (NIH-NHLBI)



High Resolution Membrane Structure from Fluorescence

Erwin London

The goal of this project will be to continue studies of the structure and function of lipid rafts: ordered sphingolipid and cholesterol-rich membrane domains found in mammalian and other eukaryotic cells. Among other functions, rafts are implicated in sorting of proteins and lipids between membranes, signal transduction, and some types of bacterial and viral infections. Previous studies in this project, as part of a (continuing) collaboration with the lab of Dr. Deborah Brown (Stony Brook), established some of the basic principles explaining how sphingolipids, sterols and certain proteins form rafts. New fluorescence and fluorescence quenching methods allowing detection nanoscale rafts with full control over raft composition, combined with previously developed spectroscopic and biochemical techniques, will be used to define several of the still mysterious rules controlling lipid and protein participation in rafts. The basis of raft formation in the sphingolipid-poor plasma membrane inner leaflet will be studied in model membrane systems. Raft-forming behavior of biosynthetic precursors of cholesterol will be studied to help define how diseases blocking steps in cholesterol biosynthesis (e.g. Smith-Lemli-Opitz disease) may be related to deleterious changes in raft behavior. Ceramide displaces sterols from rafts.

For this reason, biologically important ceramide-rich rafts will be studied in model systems and cells to define how they differ from ordinary rafts in terms of properties and protein interactions. To gain additional insights into the principles of raft formation, various small molecules with raft-promoting and raft-destabilizing behaviors will be studied in model membranes and cells. As part of these studies, the functional significance of the known raft-destabilizing effects of polyene antibiotics will be studied in both model membranes and cells. The interaction of proteins with rafts will be studied to define the relationship between protein structure and raft affinity. Transmembrane. lipid-anchored and cholesterol-binding proteins will be compared. Sterol analogs found to support raft formation to different degrees in the last grant period will be used to define the nature of protein sterol binding specificity. Whether proteins interact differently with ordinary and ceramide-rich rafts will also be determined. Finally, the degree to which proteins can regulate raft formation will be studied. (NIH)

Structure & Dynamics in Colloidal Polyelectrolyte-Surfactant Complexes

Ben Chu, C. Burger, M. Hadjiargyrou

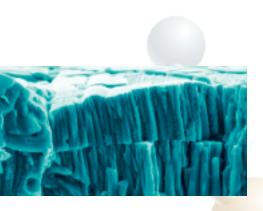
Experiments involve the synthesis of multi-functional copolymers with different architecture, chain length and chain ratio, as well as studies of the complex formation with DNA in both organic and aqueous media. Graft tri-functional copolymers based on chitosan and tri-arm block copolymers composed of polyethylene glycol, polylactide and poly(L-lysine) have already demonstrated their feasibility in initial studies. The copolymer composition will be controlled by changing the reaction conditions and feed ratio. In order to endow the copolymer with a pHresponsive property, a novel copolymer. which can transform amphiphilic polycations to polyanions, will be synthesized. The complex formation between DNA and copolymers, and the supra-molecular structure, will be investigated mainly by laser light scattering, transmission electron microscopy (TEM), synchrotron small angle X-ray scattering (SAXS) and electrophoresis. (NSF)



Helmut Strey

The project is aimed to investigate the role of electrostatic forces in the assembly of biological materials such as proteins, DNA condensation inside sperm heads, and formation of arterial plaque. The proposed research is strongly motivated by the richness of materials found in nature often displaying superior mechanical properties and functionalities. Under this project, biological molecules (peptides and proteins) will be combined with synthetic macromolecules (specific electrolytes and copolymers) to create novel functional hybrid materials with superior properties and performance. The results of this work impact the basic understanding of biological self-assembly processes and contribute to applications in the biotechnology and pharmaceutical industries. Our project is highly interdisciplinary and will train students and postdoctoral researchers in the increasingly complex interdisciplinary work in science, engineering and medicine. Our team members will acquire skills in state-of-the art microscopy, synchrotron X-ray scattering at national laboratories, and biochemical methods to prepare them for careers in academia, government and industry.

The project will investigate electrostatically self-assembled materials. In particular, we will focus on complexes of charged objects (membranes, cylinders and spheres) with oppositely charged polyelectrolytes (PE) or tri-block copolymers (PEneutral-PE). With this strategy, we expect to create functional hybrid materials from building blocks that are taken from biology (peptides and proteins) and synthetic polymer chemistry. By systematically varying the interaction strength and range between building blocks we will identify conditions for longrange order. The results of this work will not only impact the basic understanding of biological selfassembly processes, but also through extension to material science contribute to applications of self-assembled nanostructured materials in drug delivery, tissue bioseparation engineering. processes, biosensor materials, novel filter materials, as well as fuel cells. The interdisciplinary nature of the project will produce students and postdoctoral researchers that have a rigorous science background, are independent thinkers, and have an understanding of intellectual property and real world applications; all those aspects being highly valued by industry as well as academia. (NSF)



Electrostatic Potentials and Biological Membranes

Stuart McLaughlin

The long term objective is to understand how physical factors (electrostatics, diffusion, reduction of dimensionality) produce a flow of information through calcium/ phosphoinositide second messenger systems. Phosphatidylinositol 4,5-bisphosphate, PIP2, is the source of three second messengers and is involved in a wide range of membrane-related phenomena, such as the activation of ion channels or enzymes, endocytosis, and exocytosis. How does PIP2 do so much? The working hypothesis is that unstructured clusters of basic/hydrophobic residues on MARCKS and other proteins act as reversible PIP2 buffers: they produce a local positive electrostatic potential that sequesters the polyvalent acidic lipid. Upon a local increase in the level of Ca2+, calcium/calmodulin (Ca/CaM) binds to the cluster, releasing the PIP2. Six specific aims will explore this hypothesis.

First, a simple coloring scheme and peptide binding measurements will be used to identify basic/hydrophobic clusters on medically important proteins. This approach has allowed the PI to identify regions of interest on receptor tyrosine kinases (RTK), G protein coupled receptors, and scaffolding proteins that are important in cancer and as drug targets.

PCS, FRET, fluorescence stop flow, and other measurements will be used to determine peptide affinity for membranes, Ca/CaM, and PIP2. The biological consequences of these interactions will be investigated in collaborations with cell biologists. The recent identification of three such clusters on gravin illustrates the power of the combined biophysical/cell biology approach.

Second, to use fluorescence measurements to determine the kinetics and life time of Ca/CaM binding to reconstituted peptides corresponding to the basic/hydrophobic juxtamembrane + transmembrane regions of intrinsic membrane proteins. Third, to determine how unstructured basic clusters provide sufficient specificity for PIP2 to target proteins such as the sperm factor PLC to the plasma membrane. Fourth, to test the postulate that GAP-43/neuromodulin acts as a reversible PIP2 sink in the axonal growth cones of neurons. Fifth, to show that the basic/hydrophobic peptides diffuse more rapidly than lipids when bound to membranes that lack PIP2, preventing sequestration of other lipids such as phosphatidylserine and cholesterol. Sixth, to test a model for how basic/hydrophobic regions of proteins (e.g. MARCKS, gravin, RTKs) may nucleate the formation of cholesterol-enriched rafts. (NIH)

Carbon Nanotube and Nanodot Self-assembled Layers

V. Samuilov, C. Clayton, M. Dudley, M. Rafailovich, I. Sokolov

A promising nanotechnology-related work at the Sensor CAT is led by Dr. Vladimir Samuilov (MSE Dept). His research is based on the proprietary platform technology of self-assembling of uniform monolayers of functionalized carbon nanotubes (patent applications are pending). Over the last 5 years, the following directions have been investigated:

- Carbon nanotube based sensors. Gas sensors for H2, CO2, H20. (SBDC, SBU Sensor CAT, SPIR)
- Carbon nanotube coating for heat dissipation. (SBDC, SBU Sensor CAT, SPIR)
- Electrospinning technique for nanosensor application. (SBDC, SBU Sensor CAT, SPIR)
- 4) Self-assembled 2-D arrays of metal nanocrystals and the fabrication of highly ordered arrays of metallic nanoparticles. (SBDC, SBU Sensor CAT, SPIR)
- 5) DNA Separation and Single DNA Molecule Sequencing using a nanoscale integrated device. (NSF, SBDC)
- 6) Novel method of DNA arrays electrical readout on nanostructures. Collaboration with BNL (Center for Nanomaterilas and Bio Department) and with Cat for Biotechnology

Nanoscale Control Of Biological Phenomena

Richard A.F. Clark, Miriam Rafailovich, Nadine Pernodet

Understanding the construct of actual tissue in vivo requires the ability to arrange cells in three dimensions on a scaffold that can allow for tissue regeneration. In this section the fundamental issues are

- Engineering porosity on various length scale to enable cell proliferation or differentiation as well as molecular diffusion enabling for genomic transvection, PH, and control of electrolyte.
- 2) Incorporate chemical heterogeneity that allows for integrin binding which enables cell mobility. Here multiple length scales must be addressed since the proper placement of these sites must be known in order to control the cell diffusion rates for applications such as wound healing without scarring.
- Design mechanical rigidity so as to induce the appropriate cell morphology and allow sufficient elasticity to expose binding domains required for migration.

Several approaches will be used here. Various chemical modifications are being employed to prepare films made of Hyaluronic acid (HA), a naturally occurring biopolymer, which have found numerous applications in wound healing and as anti-adhesive barriers following surgical procedures. One such modification involves the formulation of thiolated HA (HA-DTPH) hydrogels, where the mechanical

properties can be varied by the spacing and length of the polyethylene glycol diacrylate (PEGDA) cross linker.

Furthermore, cell adhesion and migration can be facilitated by the incorporation of fibronectin, collagen, fibrin or other proteins. The effect on micro scale cell morphology by the nanoscale variation in mechanical and chemical properties can be profound. The role of each component can be studied independently by fluorescent GFP transvection of the cells and in situ observation of the cell migration.

(NSF, NIH)

The Interaction of Cells with Nanoparticles

Richard A.F. Clark, M. Rafailovich, Nadine Pernodet

Due to their large surface to volume ratio nanoparticles i.e. metallic or dendritic are increasingly being used for drug delivery, imaging, and therapy. These nanoparticles are commonly produced from materials considered non-toxic to cells plated on macroscopic surfaces. Yet when particulates are produced from the same material, the much smaller size allows them to penetrate the cell membrane where their accumulation can interfere with cell function and become toxic. Furthermore, in vivo

targeting of therapeutic and imaging agents to cells with specific phenotypes such as cancer cells and infected cells is presently limited to monoclonal antibodies generated to have binding sites for specific cell surface epitopes.

Despite "humanization" of these murine molecules by substitution of human antibody structure for all but the binding site, all widely used therapeutic antibodies are immunogenic. The resulting toxicity limits repeated use and renders them unsatisfactory for routine screening for disease. We therefore propose the following:

- A systematic study will first be performed where we will try to isolate only the effect of shape and dimension on toxicity.
- 2) We will experiment with different mechanisms for enabling specificity and efficient delivery while minimizing toxcity. For example, nanoparticles can be derivatized with epitopes for cells of particular phenotypes, which would be immunologically non-reactive.

In order to determine the location of the epitope on the cell membrane, the particles will be attached to an AFM tip which will then be used to provide a force distance map of the cell surface. Through this mechanism we hope to be able to identify specific loci that will differentiate between normal or cancerous cell types. (NSF, NIH)

Nanotechnology in Medicine

Materials for Bioseparation, Drug Delivery and Biosensors

Helmut H. Strey

Nature's ability to assemble simple molecular building blocks into highly ordered materials, such as those found in cell membranes. cell nuclei, cytoskeleton, cartilage, or bone presents many fascinating and unanswered questions. We are interested in how to tune the interactions of water-soluble building blocks so as to induce their selfassembly into useful microstructures much needed for the next generation of controlled drug delivery, biosensors and DNA sequencing applications. Such materials, because of their well-ordered porous structure, will allow more efficient molecular separation and drug delivery. The biosensors should be able to quantitatively detect and measure analyte concentrations at hormonal levels. (NSF, DOE)

Early Noninvasive Detection of Colon Cancer Recurrence Using Nanosensors

Basil Rigas

Colon cancer is one of the leading fatal malignancies in the western world. While surgical removal of the primary tumor is often feasible, recurrence remains a significant problem and to a large extent it determines the outcome of the patient. We propose to use nanosensors to aid in the early detection of cancer recurrence in the colon. The principle of this approach is the following: During surgery for tumor excision sensors are implanted in the remaining colon that detect the levels of an analyte, such as CEA that signifies recurrence. Most sensors will be at the anastomosis site, which is the most frequent site of recurrence. At certain time intervals the sensor is activated remotely to obtain a reading of the levels of the analyte of interest in the colonic mucosa. If the result indicates recurrence. the colon is explored either via endoscopy or other appropriate means. (NIH)

Opportunities for Applied Nanotechnology in Medical Practice

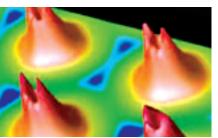
Mary (Molly) Frame

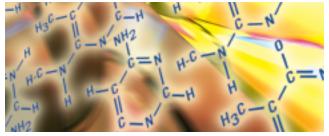
Nanotechnology has the immense potential to positively impact health care within the next decade. Although nanoscience as a field is largely in the discovery phase, many areas of nano-based research at Stony Brook University and Brookhaven National Laboratories are close to a translational step. Broad areas of research include targeted drug delivery vehicles, scaffolding for organ specific tissue engineering, biosensor lab-ona-chip for molecular detection or DNA separation, and the long-term effects of nanomaterials (either natural or engineered). (NIH)

Long-term Biocompatibility

Mary (Molly) Frame

In conjunction with many of the projects described above, ongoing efforts examine the effect of chronic exposure to natural or nanoengineered materials. This includes verification of whole animal and cellular compatibility with quantum dots (Drs. I Cohen, P Brink), and with engineered microspheres (Drs. W Chen, M Frame). Further cell culture studies examine the effects of nanoengineered scaffolding on cell viability and differentiation (Drs. M. Hadjiargyrou, M Frame. Entcheva). Important environmental studies examining the molecular basis for contamination by natural or nanoengineered systems are underway by several groups (Drs. G Halada, M Schoonen, S Tsirka and others). (NIH)





Synthetic Viral Genome Design for Rapid Vaccine Development

Steven Skiena and Eckard Wimmer

Based on our prior experience with the de novo genome synthesis of attenuated polioviruses (Cello et al. 2002, Mueller et al 2006) we will use new computer based algorithms to design and de novo synthesize viral genomes. These will encode exactly the same proteins as wild-type viruses, but by using alternative, synonymous codons, we will alter codon bias, codon pair bias, RNA secondary structure, dinucleotide content, and other parameters. Our past experience has shown that these coding-independent changes produce highly attenuated viruses, often due to poor translation of proteins. By targeting an elementary function of all viruses, namely protein translation, we hope to develop a very general method for predictably, safely, quickly and cheaply producing attenuated viruses, which will then be useful for making vaccines. Initial development will take place in the very well understood model system poliovirus, but we will move on to other viruses (e.g. influenza) where there is a medical application. (NSF, NIH)

Electrospinning of Hyaluronan Scaffolds

Ben Chu

Tissue engineering technologies offer the promise to treat a wide variety of injuries and diseases. The project aims at investigating cardiovascular tissues, where there has been only limited progress towards regenerating complex matrix structures vital to tissue homeostasis. A part of the problem has been that cardiovascular tissues are far more complex than initially envisioned and have a capacity for self-repair that is far less effective than tissue-engineering principles demand. An outstanding problem addressed by this study is to manufacture structurally- and functionally-faithful vascular elastic matrices on demand. Elastin is crucial to maintaining native structural configurations of tissues and regulating cell signaling pathways involved in morphogenesis, injury response, and inflammation. Efforts will be made to regenerate lost elastin structures in vivo. Tissue engineered constructs have thus far been limited by the progressive destabilization of tropoelastin mRNA expression in adult vascular cells and the unavailability of suitable scaffolding materials to provide the cellular cues necessary to up-regulate elastin synthesis. Our task is to regenerate nanofibrous matrices that are structurally- and functionally-faithful mimics of native elastin. (NIH)

Targeted Delivery

Mary (Molly) Frame

Targeted drug or stem cell delivery is the goal for wound healing, cancer treatments, cardiac repair or diabetes treatment. Specific research projects related to wound healing examine biodegradable microspheres or hydrogel bandages (Dr. W Chen), novel extracellular matrix hydrogels (Dr. R Clark) and polymeric nanocomposites and electrospun materials with imbedded antibiotics (Drs. B Chu, B Hsiao, M Hadjiargyrou). Targeted cancer treatments include the use of caged substrates for matrix metalloproteases using nano-driven imaging for long term monitoring (Dr. H Crawford). Quantum dots (QD) are used to determine the fate of human mesenchymal stem cells (hMSCs) in cardiac repair by loading the stem cells with QD, and monitoring their eventual differentiation (Drs. I Cohen, P Brink and others). Both cardiac myocytes and vascular endothelial cells are found with QD after several weeks (Figure 1). (NIH)

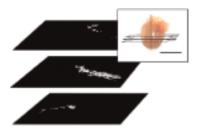


Figure 1. Rat hearts were injected with QD-hMSCs. Fixed, frozen sections were cut transversely (as shown in inset) at 10-lm and mounted onto glass slides. Sections were imaged for QD fluorescence emission (655-nm) with phase overlay to visualize tissue borders. Serial low power images were registered where white pixels depict the QD-positive zones in the images. [Figure from: Rosen, et al., in press, http://www.StemCells.com.]

Angiogenesis Induced by a Biodegradable Nanoparticle VEGF DNA Delivery System

Weiliam Chen

Recent in vivo experiments have demonstrated that a biodegradable nanoparticle formulation intended for prolonged VEGF DNA delivery is capable of inducing angiogenesis in hindlimb muscle 4, 12 and 18 weeks after injection. This sustained DNA delivery system will ensure the continual presence of VEGF to facilitate the maturation of newly formed blood vessels and thus their persistence. The VEGF DNA microparticles will be used to induce angiogenesis in porcine chronic ischemic myocardium. (NSF)

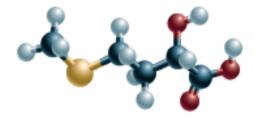
Nanomechanical Properties of Biological Tissue and its Application in Regenerative Medicine

Yi-Xian Qin

Despite having been studied for quite some time, however, the mechanical behavior of trabecular bone tissue is surprisingly difficult to understand. A large part of this stems from the fact that the technology to study trabecular bone's tissue mechanical properties has only relatively recently become available in the form of nanoindenters adopted from traditional hardness testing for geologic and materials testing applications. The trabecular mineral concentration has been previously shown to be constant throughout life such that the reduction in apparent modulus and strength is due to loss of substance without concomitant loss of tissue quality.

The purpose of this study is to gain a preliminary understanding of these properties and their interrelationships. As such, trabecular tissue and other biological tissues from healthy and diseased animal and human will be studied using a nanomechanical assessment using nanoindentation. In the preliminary tests, the local variability is thought to be quite important for its influence on the apparent level mechanical behavior in the tissue. This will provide further evidence that nano-scale property of biological tissue can provide information for early diagnostic and treatment outcomes.

Furthermore, the objective of this study will also be to analyze the respective effect of microstructure and material properties on the ability of linear elastic μFEM to assess apparent mechanical behavior using trabecular bone samples with known apparent and nanomechanical properties. The finite element solver chosen for this study was the relatively newly available iterative solver packaged with the image processing language of the Scanco µCT systems. There are two important benefits of this system. In particular, this approach can potentially be used for predicting in vivo bone strength in the future when in vivo µCT becomes available for human use. (NIH)



Nanotechnology in Materials

Tissue Engineering

Mary (Molly) Frame, Emilia Entcheva, Perena Gouma

Established collaborations in the field of tissue engineering study cardiac, vascular and bone scaffolding for implantation. In addition to cardiac repair in a whole animal model (Figure 1), de novo cardiac tissue engineering is examined on micro-patterned topographical surfaces to understand the relationship between cardiac signaling, contraction and the interaction of the cells with their substrate patterned (Dr. Entcheva). Using electrospun scaffolding a template for de novo capillary network growth has been constructed (Figure 2, Drs. M Frame, P Gouma). Combining micropatterned topographical cues and nanostamped chemical surface modifications, in a novel bioassay chamber, this microvascular tissue engineering project is capable of creating autologous grafts for rapid re-vascularization of wounds.

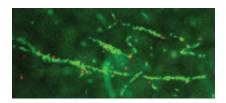


Figure 2. Spontaneous capillary network structure formed by human umbilical vein endothelial cells on electrospun scaffolding. Cells are calcein (live, green) and ethidium (dead, red) stained. Rapid time to confluence is achieved by guiding endothelial cell growth patterns. [Image from: Rubenstein, et al., in press, Microcirculation.]

Electrospun scaffolding is additionally being used as a hard tissue growth template (bone) in which DNA or other bioactive molecules are imbedded to enhance specific mitogenic activity (Dr. M Hadjiargyrou and others). (NIH)

Nanostructured Thin Silicon

Charles Fortmann

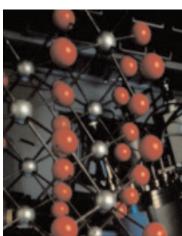
This project is investigating the use of nano-engineered silicon structures for site specific pharmaceutical delivery. This project spans the range from theoretical material engineering to actual material generation. It involves an agent simulation of the life cycle that abandons the deterministic rate equation approach to model various cel-Iular cyclic systems (metabolic cycle) using independent, nondeterministic agents performing the various interconnected: reactions, diffusion, energy production and feedback circuits. (Solar Physics Corp.)

Risks of Introducing Nanomaterials to the Clotting and Inflammatory Systems

Jolyon Jesty

We have particular expertise in the area of clotting and inflammation. Clotting: introducing foreign materials is clearly an enormous risk, especially for activation of clotting via the contact system. We can measure activation of clotting by different methods at least as well as anyone else. Inflammation: Nanomaterials are so small that they will almost certainly get taken up by endothelial cells (ECs), and the ECs play a major role in the initiation of the inflammatory response (involving the platelets as well). Both ECs and platelets are intimately tied in with the clotting system. (NIH)





Micro/Nano Mechanics: Studies of Sandwich Foam Composites

Fu-pen Chiang

Sandwich foam composites are light weight high strength structural materials. They are ideal materials for building high speed coastal patrol boats. This project investigates the micro mechanical properties of foam materials using a unique measuring technique called Inter-ferometry Speckle Electron Microscopy which can provide strain distribution in an area only a few microns in size. By mixing a small portion of nanoparticles into polymeric foam, the resulting material has a higher stiffness and also retards flame. Studies are being carried out on both the pure and the nanophased foam materials. (ONR)

Modeling Dissipative Mechanisms in Nanoscale Systems

Dilip Gersappe, George Stell and Phil Allen

Molecular dynamics simulations would seem to be the obvious computational method of choice with which to study the failure mechanisms of these more complex polymer nanocomposites. When these simulations are used in isolation, however, the exhaustive search required to isolate the critical variables can become computationally

prohibitive. Mean field theories, too. are limited by their inability to calculate partition functions or probability distributions due to the complexities of the nanostructured environment. Used in conjunction, however, these methods offer the possibility of bridging the gap between the meso and the nano scales. The methodology that we plan to use is to use a series of models that operate at increasingly larger length scales. The principle is that the finer grained models will provide the parameters for the more coarse grained models. We plan to start by using MD simulations on detailed systems. Potentials for the MD simulations will be determined from atomistic calculations on the filler particles. These results will allow us to formulate statistical mechanical models to investigate the thermodyproperties of polymer nanocomposites and determine conditions under which there is a percolating network of nanofiller particles. Finally we will design a dynamic mean field model that will investigate the effect of shear on the properties of the nanocomposite and also continuum mechanical models to study the effect of tensile strain in these systems. We also plan on extending this methodology to more complex nanocomposite morphologies such as nanofoams and nanofibers. (NSF, NIH)

The Structure of Several Natural Nanomaterials

Martin Schoonen

Over the last few years we have resolved the structure of several natural nanomaterials using total X-ray scattering techniques. In essence, we have been able to shed light on the structure of several materials that had been characterized as X-ray amorphous. The new structural information allows us to better understand reactivity, transformations, interaction with contaminants as well as other parameters. There may be some future environmental applications, but that has not been the focus at this point. The latest of these effort has led to a paper in Science. Michel FM, Ehm L, Antao SM, Lee PL, Chupas PJ, Liu G, Strongin DR, Schoonen MAA, Phillips BL, Parise JB (2007) The structure of ferrihydrite, a nanocrystalline material. Science 316:1726-1729. (NSF)

Oxide Nanomaterials for Energy Applications

Stanislaus Wong

We have been focused on several key nanoscience issues. We have a strong effort in the chemical functionalization of carbon nanotubes. and a growing program in the synthesis and characterization of nanoscale metal oxide materials, related to energy applications. Examples include the following:

1) Three-dimensional, dendritic micron- scale spheres of alkali metal hydrogen titanate 1D nanostructures (i.e.: nanowires and nanotubes) have been generated using a modified hydro thermal technique in the presence of hydrogen peroxide and an alkali metal hydroxide solution. Sea-urchin-like assemblies of these 1D nanostructures have been transformed into their hydrogen titanate analogues (lepi docrocite HxTi2x/4 fix/404 (x~0.7, fi: vacancy))by neutralization as well as into their corresponding anatase TiO2 nanostructured counterparts through a moderate hightemperature annealing dehydration process without destroying the 3D hierarchical structural motif. The as-prepared hollow spheres of titanate and titania 1D nanostructures have overall diameters, ranging from 0.8 £gm to 1.2 £gm, while the interior of these aggregates are vacuous with a diameter range of 100 to 200 nm. We have demonstrated that these assemblies are active photocatalysts for the degradation of synthetic Procion Red dye under UV light illumination.

2) A size- and shape-dependent morphological transformation was demonstrated during the hydrothermal soft chemical transformation, in neutral solution, of titanate nanostructures into their anatase titania counterparts. Specifically, protonic lepidocrocite hydrogen titanate nanotubes with diameters of ~10 nm were transformed into exceptionally high-purity anatase nanoparticles with an average size of 12 nm. Lepidocrocite hydrogen titanate nanowires with relatively small diameters (average diameter range of T 200 nm) were converted into single-crystalline anatase nanowires with relatively smooth surfaces. Larger diameter (>200 nm) titanate nanowires were transformed analogous into anatase nanowire motifs, resembling clusters of adjoining anatase nanocrystals with perfectly parallel, oriented fringes. Our results indicate that as-synthesized TiO2 nanostructures possessed higher photocatalytic activity than the commercial titania precursors from whence they were derived. (DOE, Batelle)

Polymer-Assisted Formation of Nanostructured Transition Metal Clusters and Crystals

Ben Chu

To produce nanostructured transition metal clusters and crystals, like polyoxometallates and in particular polyoxomolybdates, the role of different reducing agents and different transition metals (like molybdenum and tungsten) starting species and the nature of the reduction-oxidation (redox) processare investigated. A new approach is being proposed in the nano-fabrication of these clusters with emphasis on ordered inorganic nano-structures, by investigating the delicate control on the redox potential of oxidation-reduction reactions for the reactive species responsible for the final transition metal structures with nano-scale modifications. The proposed study aims to investigate more specifically the formation of cluster (e.g., polyoxomolybdates) using controls on the redox potential, together with a range of other parameters, such as the nature of the reducing agent, pH, ionic strength, nature of ionic species, and the subsequent crystal growth in confined geometry in the presence of polymers as a modulating agent so that a more generalized understanding can be formulated, not only on existing forms of polyoxomolybdates but also leading toward new pathways on the polymer-assisted formation of new inorganic structures. (DOE)

Nanotechnology in Electronics

Lab-On-A-Chip

Mary (Molly) Frame, Helmut Strey, Perena Gouma, Stanislaus Wong

Multiple approaches are currently being used to nanofabricate biosensors or diagnostic chips. Nanochannels guiding strand DNA were developed for DNA hybridization and gene typing (Dr. H Strey). Biocomposites for selective chemical sensing were fabricated from a hybrid leucoemeraldine-polyaniline; these "nano-noses" detect minute gaseous pollutants (Dr. P Gouma). This lab has further developed a biosensor chip for detection of thrombosis (Dr. P Gouma). Other biosensors include effective design of chemical or biological catalysts based on unique self assembly properties and novel use of carbon nanotubes (Dr. S Wong). Self assembly of gold-protein sheets are showing promise for use in detection of and deactivation of lethal bacteria, such as drug resistant tuberculosis (Drs. H Li, J Hainfield, L Qian, E Lymar). (NIH)



Figure 3. A cryo-electron micrograph showing a single layer of evenly spaced enzyme structures (colorful "wheels") interspersed with gold nanoparticles (magenta). [Image from: http://www.bnl.gov/cfn/news/PRdisplay.asp? prID=07-73]

Extremely Low-Power Hybrid Silicon/ Nanoelectronic Circuits

K. Likharev

We have proposed a new approach (dubbed "CMOL") to the reduction of power consumption in microelectronics. In this approach, a silicon chip is augmented by a simple add-on nanowire circuit ("crossbar""), with two-terminal nanodevices formed at each crosspoint. (Reliable fabrication of nanodevices of the required "programmable diode" functionality has already been demonstrated by electronic industry in the context of their memory applications.) The crossbar is connected to the semiconductor transistor base via a pinbased interface distributed all over the chip area. Our simulations have shown that digital CMOL circuits may reduce power consumption of semiconductor chips by at least two orders of magnitude (at the same performance) and thus contribute very significantly to energy conservation. Our plan include experimental demonstration, within the next few years, of the first operational CMOL chips. (AFOSR, DRO, MARCO, NSF)

Hybrid CMOS/Nanoelectronic ("CMOL") Circuits

K. Likharev

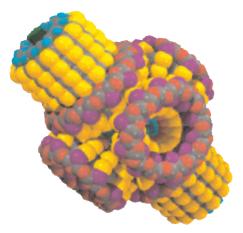
The main focus of our work is the conceptual development, as well as experimental and theoretical studies of various aspects of future hybrid CMOS/Nanoelectronic ("CMOL") Circuits for a broad range of applications. Preliminary calculations have shown that CMOL circuits may enable:

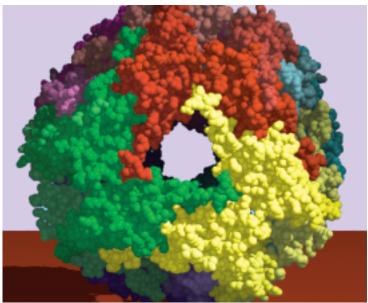
- terabit-scale memory chips and embedded memories,
- reconfigurable FPGA-like logic circuits with a ~100X density advantage over similar CMOS circuits, and
- mixed-signal circuits for advanced information processing with unprecedented performance (up to 1020 elementary operations per cm2 per second), at manageable power consumption and high defect tolerance.

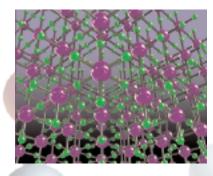
The group's work, conducted within a multi-disciplinary, SBU-led collaboration, includes the following components:

- fabrication of novel, single-electron molecular devices (in collaboration with groups led by Prof. Dilip Gersappe of Material Sciences, Prof. Jim Lukens of Physics and Astronomy, and Andreas Mayr of Chemistry),
- experimental study and theoretical analysis of electron transport through such molecules (in collaboration with Prof. Phil Allen of Physics and Astronomy and the group led by Dr. Mark Pederson of the Naval Research Laboratory),
- development of novel architectures for CMOL circuits (in collaboration with Prof. Paul Adams of Neurobiology and Behavior, Dr. Jacob Barhen of ORNL, and Dmitri Strukov of HPL), and
- experimental demonstration of first CMOL circuits (in collaboration with Prof Jim Lukens, Prof. Michael Shur of RPI, Prof. Wei Wang of Purdue/ Indianapolis, and industrial partners).

(AFOSR, DTO, MARCO, NSF)







Nanotechnology in Chemical Sensing

Nanotechnology and Chemical Sensing

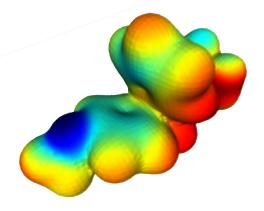
Perena Gouma

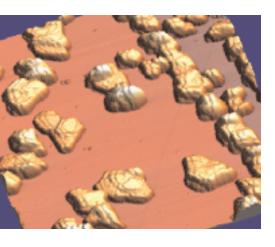
The group has developed various nanosensors utilizing single crystal metal oxide nanowires and hybrid organic and inorganic systems for the detection of chemical as well as Biological species. We have also built electronic nose-type technologies, comprised of small sets of highly specific gas sensing elements. Finally, we are using these sensors as occupancy sensors can reduce energy use by as much as 45%. Improving energy efficiency can reduce emissions that contribute to global warming, mercury contamination in lakes, acid rain, and nuclear waste. (NIH)

Selective Electronic Noses for Medical and Homeland Security Applications

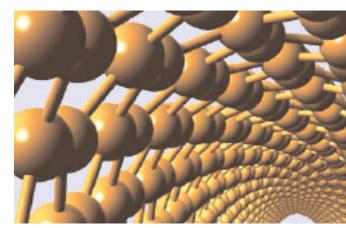
Perena Gouma

This project involves the development of advanced, selective chemosensor arrays for the detection of chemical\and biological warfare agents as well as for the fabrication of sensing probes for breath analysis of pathogens. The elements we use are nano-composite metal oxides and bio-doped materials. (NIH)









Nanotechnology in Energy

Environmental Nanotechnologies for Clean Energy Applications

Gary Halada

To truly understand interactions between the environment and natural and man-made materials, it is essential to understand reactions at the nanoscale. It is at this level, from single molecules to ultra-thin films on surfaces, that structural and chemical transformations first occur which affect critical environmental processes, such as corrosion of advanced alloys, association of hazardous waste with soil or buildings, and transformation of radioactive materials by microbes. In addition, to create the next generation of materials and technologies to solve critical environmental problems we need to create new methodologies and research partnerships that will provide the necessary combination of tools, software and knowledge for crossdisciplinary problem-solving. Examples of our ongoing research include:

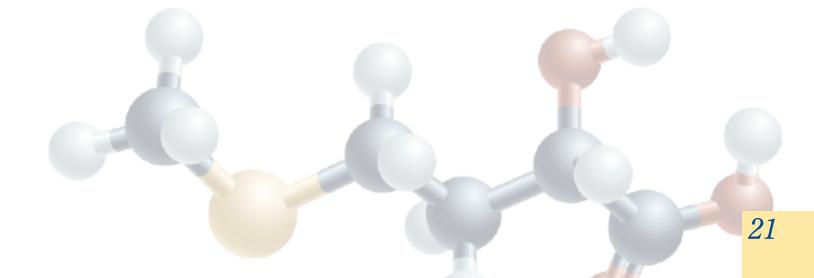
- 1) Optimizing radioactive clean-up technologies through modeling the effect of electron transfer on uranium-organic complexes
- 2) Using functionalized carbon nanotubes in ultrasensitive electrochemical sensors
- 3) Developing new safe and effective technologies for remediation of contaminated structures
- 4) Characterizing the interaction of toxic metals with biomacromolecules to better understand the nature and fate of mixed waste
- 5) Studying the chelation of pollutants through state-of-the-art quantum mechanical molecular modeling and density functional theory
- 6) Using photochemical reactions on iron nanoparticles for environmental remediation.

(NSF)

Molecular Engineering, the Next-Generation Gas Separation Technology

Devinder Mahajan

Natural gas upgrading is a major challenge once gas fields are identified. Raw gas needs upgrading by removal of gases such as CO2 and N2 that are naturally found mixed with CH4. Our two distinct approaches are as follows. In the first approach, the molecularly imprinted polymer (MIP) membranes are being produced using a process based on rapid precipitation from a supercritical solution followed by vapor treatment and UV photo polymerization. The material pore size is tuned to the template vapor but without chemical functionality to achieve high selectivity in natural gas purification. In the second approach, polymers such as polystyrene (PS) are being modified with supercritical CO2 to control the pore size of the polymer for enhancing gas separations. The goal is to identify polymer candidates for ultimate application in natural gas fields. (BNL, (DOE)



Nanofibrous Membranes for Energy Applications

Ben Chu and Benjamin S. Hsiao

Our research group is currently focused on the development of unique nanoscale fabrication methods, i.e., multiple-jet electrospinning and electro-blowing processes, to produce nanofibrous membrane materials for industrial and biomedical applications. The existence of this platform technology now permits us to seriously consider the great potential in its unique ability to manipulate functional materials at micro- and nano-length scales. The key innovative features of our multiple-jet electro-spinning/-blowing technologies are as follows:

- 1) extremely high surface to volume ratio;
- 2) variation in porosity, pore size, pore size distribution and nanoscale fiber diameter;
- 3) multiple-functionality and surface modification;
- 4) durable mechanical strength and
- 5) construction of unique hierarchical structures, including pattern formation with composites materials.

The proposed research aims to design, develop and create new nanostructured materials for energy storage device applications by combining the multiple-jet electro-spinning/-blowing technology with novel chemical and physical pathways to prepare functional organic/inorganic nanocomposite membranes.

The new format should have unique electrical conducting and mechanical properties as well as tailor-designed functionality, with immediate applications to battery (e.g. new anodes and cathodes) and fuel cell (e.g. catalyst support membranes) development. (NIH)

High-Flux Low-Fouling Membranes for Bilge-Water Filtration

Ben Chu

The project aims to investigate several fundamental issues of a breakthrough technology on high-flux loe-fouling water purification filters being developed at Stony Brook. This breakthrough technology is based on a new concept of composite membrane design, involving (1) the replacement of conventional flux-limited porous membrane layer with a high flux non-woven nanofibrous support, containing an asymmetric structure with interconnected void morphology, and (2) the coating of a very thin barrier layer of strong and functional polymer nanocomposite on the nanofibrous scaffold. Preliminary experiments on the hierarchical structure of the design and assembly of this unique nanofibrous nanocomposite membrane, with or without the mid-layeer support, have already revealed very promising potential (e.g. by using a nonporous hydrophilic nanocomposite coating top-layer, an asymmetric electrospun nanofibrous mid-layer and a conventional non-woven microfibrous support, the flux rate of several such not yet optimized systems, is already 5-10 times more than that of the best among conventional UF media with comparable rejection ratio and low fouling criteria. (ONR)

Novel Sensors for Harsh-Environment Energy Generation

Jon Longtin

Direct-Write Thermal Sensors fabricated using thermal spray technology have several unique advantages over traditional sensors that have to be mechanically attached to engineering components. The unique microstructure nanometer-scale features associated with thermal spray coatings, including pores and cracks, voids, the presence of many splat-splat interfaces and micro cracks all result in unique thermal, mechanical, and electrical properties that result in excellent performance at very high temperatures (1000+ oC) and in harsh environments. These sensors can be fabricated directly onto engineering components for outstanding reliability. A key application for these sensors is their use in land-based turbines and hightemperature, high-pressure boilers for more efficient power generation, condition-based (vs. failurebased) maintenance, and optimal performance. The work is funded by federal and industrial sources. (NSF)

Instrumentation Development on Multi-Scaled Scattering for Bio-Molecular Solutions

Ben Chu

The project is aimed at incorporating the newly developed cross-correlation light scattering capability with synchrotron X-ray scattering, specifically designed for biomacromolecular gels, solutions and suspensions. The combined X-rays and laser light scattering techniques will be able to detect structural variations and dynamics in a continuous and very broad spatial range (0.1 - 2000 nm), even in turbid media. It is noted that many bio-macromolecular fluids, when undergoing structure changes or reactions, become opaque and multiple scattering sets in. The cross-correlation technique can extract single scattering information in relatively turbid media, while dynamic cross-correlation function analysis can yield knowledge on diffusive and rotational motions of species, including estimates of size distributions. Such

information, when simultaneously combined with X-ray scattering and diffraction results, is not attainable by conventional more popular methods such as NMR or microscopy. To make efficient usage of this instrumentation, the developed laser light scattering instrument module (with capability for single photon correlation and multiple photon cross correlation as well as angular dependence measurements) will be designed to function independently, in the absence of synchrotron X-rays. The X-ray-collimator has been designed and constructed. It is being tested the Advanced **Polymers** at National Beamline at the Synchrotron Light Source, Brookhaven National Laboratory. (NIH)





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