USC University of Southern California

USC Viterbi
School of Engineering

CHEMICAL ENGINEERING

MATERIALS SCIENCE

PETROLEUM ENGINEERING

Mork Family

Department of Chemical Engineering and Materials Science

A Message from Steven Nutt, Department Chair

The mission of the Mork Family Department of Chemical Engineering & Materials Science (MFD) is to provide our graduates with a well-rounded engineering education to meet the needs of industry, academia, and government labs; to conduct pioneering research; and to play an integrating and leadership role to the multi-disciplinary community of science and engineering.

The MFD is one of 8 engineering departments at USC. With 22 full-time faculty members and 14 joint appointees, we strive to become one of the premier departments in the world. We offer in-depth educational instruction over the full spectrum of chemical engineering, materials science, and petroleum engineering.

The reputation of the MFD for excellence in chemical engineering, petroleum engineering, and materials science is evidenced by internationally recognized scholarly work, leadership in the profession, and the education of a diverse group of highly qualified and well-placed graduates.

The MFD will foster and cultivate synergies between the three degree programs to further research and development in energy production and delivery, nanotechology, biochemical processes and medical devices. With expertise in advanced materials, and computational simulations and methods, the MFD will lead the development of cross-disciplinary synergies that serve citizens worldwide with profound scientific, technological, social, and humanitarian advances. We aim to address emerging needs of our increasingly complex and interconnected world.

I am honored to become the second chair of the MFD, succeeding Theo Tsotsis, who skillfully served as the inaugural chair of our department for the past six years. With gratitude to Theo and to my faculty colleagues, I look forward to the challenges that lie ahead, and to building excellence in all aspects of our activities.

We welcome your application to join us for graduate study in this unique and vibrant environment.

About the Department

Core faculty members: 25
Adjunct faculty: 11

Masters students (approx.): 400
PhD students (approx.): 121

Annual degrees awarded (2011-12):
- MS: 93
- PhD: 13

Average time to graduate:
- MS: 1.8 years
- PhD: 4.6 years

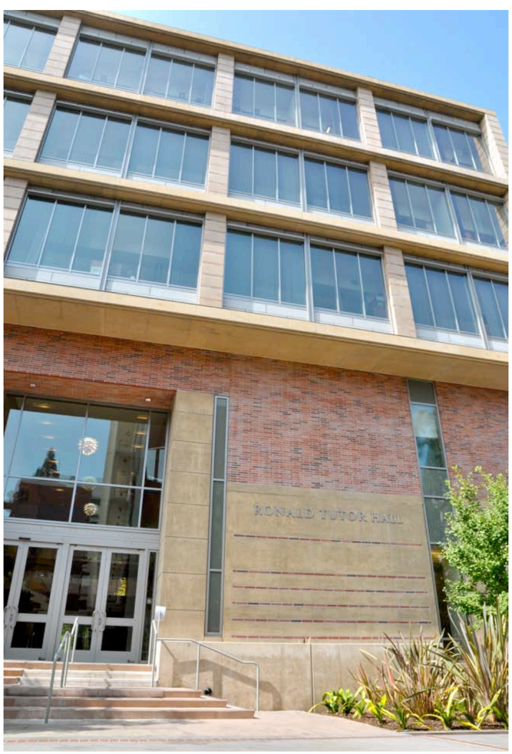
Graduate degrees offered:
- MS in Chemical Engineering
- MS in Materials Science
- MS in Petroleum Engineering
- PhD in Chemical Engineering
- PhD in Materials Science
- PhD in Petroleum Engineering

Infrastructure for Research and Teaching

The Mork Family Department of Chemical Engineering and Materials Science occupies nearly 45,000 ft^2 of lab and office space on the beautiful University of Southern California University Park Campus. This space is distributed through four buildings:

HEDCO Petroleum and Chemical Engineering Building

Neely Petroleum and Chemical Engineering Building



Ronald Tutor Hall

Vivian Hall of Engineering

Graduate Study at the University of Southern California

Ten reasons why USC should be your top choice for graduate study:

1. Distinguished faculty producing groundbreaking research that addresses critical issues facing our global society.
2. More than 400 highly regarded graduate and professional programs that prepare students for leadership positions in research, education and professional practice.
3. A strong emphasis on interdisciplinary research, including productive collaborations among professional schools.
4. Belief in the synergy between fundamental and applied research, as demonstrated by the ongoing work of more than 100 USC research centers and institutes, including:

    - The Center for Electron Microscopy and Microanalysis
    - Institute for Creative Technologies
    - USC Andrus Gerontology Center
    - USC Center for Sustainable Cities
    - USC/Norris Comprehensive Cancer Center and Hospital
    - NSF Engineering Research Center for Biomimetic Microelectronic Systems
    - USC Center for Neural Engineering
    - USC Photonics Center

5. A high-achieving and remarkably diverse 16,000-member graduate student body—almost half the entire USC student population. We enroll more international students than any other university in the United States.
6. Strong commitment to our core values: free inquiry; informed risk-taking and experimentation; mutual respect and tolerance; fairness and honesty.
7. A "learner-centered" approach to graduate education, fostering intellectual partnerships between faculty and students. Faculty play an active role in helping students hone their skills in locating, assessing, applying and presenting information.
8. Pioneering implementation of technology-assisted learning, from Internet communications to virtual reality and 3-D immersive environments.
9. A global outlook and an urban location in a vibrant international city where more than 200 languages are spoken.
10. Close ties with the local community, providing opportunities to gain real-world experience while making a lasting impact on human lives.

Faculty Research Areas

Advanced computation and simulations

Ershaghi
Jafarpour
Jessen
Kalia
Nakano
Madhukar
Sahimi
Shing
Tsotsis
Vashishta

Advanced materials technology

Chang
Goo
Gupta
Kassner
Langdon
Mansfeld
Nutt
Shing
Yoon

Biomolecular and cellular engineering

Armani
Crandall
Gundersen
Gupta
Lee
Madhukar
Malmstadt
Roberts
Tanguay
Thompson
Wang

Nanotechnology

Armani
Dapkus
Gupta
Lee
Langdon
Madhukar
Malmstadt
Roberts
Tanguay
Thompson
Wang
Will
Yoon

Electronic and photonic materials

Armani
Dapkus
Madhukar
Tanguay
Thompson
Yoon

Reaction and separations engineering

Malmstadt
Sahimi
Tsotsis

Energy and environmental technologies

Ershaghi
Jafarpour
Jessen
Gundersen
Madhukar
Mansfeld
Sahimi
Thompson
Tsotsis
Yoon
Yortsos

Systems and control

Qin

Transport processes

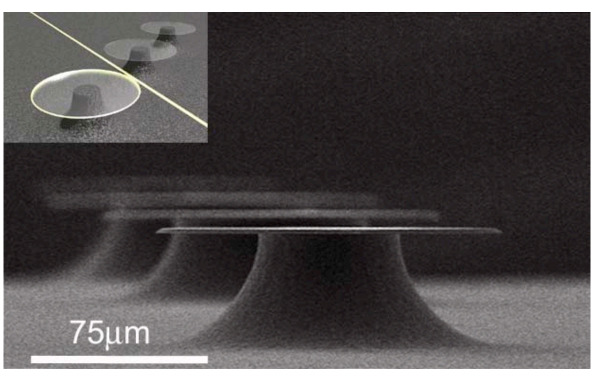
Jafarpour
Sahimi
Shing
Tsotsis
Yortsos

Andrea Armani

Biophotonics, Nanotechnology

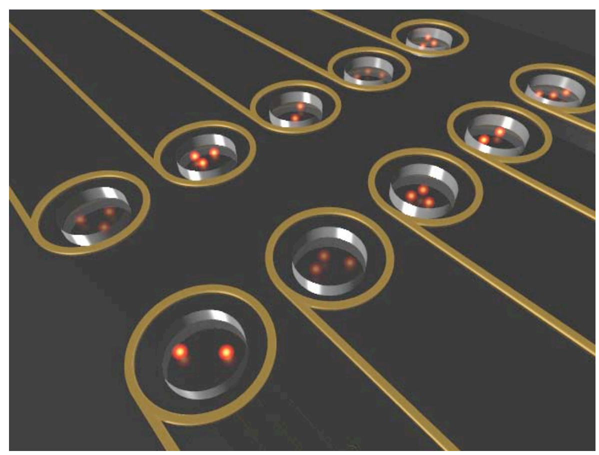
Biophotonics describes the intersection of photonics and biology. This field is very broad, covering research from chip-based microscopy to optical nano-sensors. We focus on the development and integration of optical devices for studying complex biological systems. This includes using previously characterized optical devices, such as waveguides and resonant cavities, and integrating them into microfluidics as well as conceiving and fabricating novel optical devices which have yet to be demonstrated.

One current area of research revolves around single molecule biological detection. Recent results demonstrated the ability of resonant optical cavities to detect individual molecules (see image of resonant cavity). However, the experimental measurement testing set-up and the fluid delivery is very complex. By simplifying the accompanying equipment, we aim to not only detect individual molecules, but also monitor their behavior in real-time. This will enable antibody affinity and protein folding measurements at the single molecule level. This project involves not only the optimization of the resonant cavity under study, but also the integration of the cavity with microfluidics and the stabilization of the coupling of light into the cavity. All of these efforts are secondary to the biochemistry which also must be achieved to implement the surface functionalization.



A scanning electron micrograph (SEM) of an array of silica microdisk optical resonant cavities. Inset: The optical field is confined within the periphery of the microdisk cavity (rendering performed in PovRay).

A second area of study is the integration of nano- and micro-fabrication techniques with biological imaging methods and sensing modalities. The goal is to develop a cell culture platform with integrated imaging or monitoring capabilities (see concept device). Once developed, this type of device will have applications in cell motility studies, developmental biology, and embryology. This project involves not only knowledge of biology, but also micro/nano fabrication and signal processing.



An artistic rendering of the proposed cell culture platform, in which an array of mini-incubators is fabricated, each confining between 0 to 5 cells.

As with any interdisciplinary research group, entering students are typically familiar with one area of a project, but not all disciplines involved. However, this type of research gives students the opportunity to collaborate outside of their department and to expand their academic horizons.

Return to Faculty Research Areas

Wenji Victor Chang

Polymeric Materials

Monitoring Adhesion dynamics Between Soft Materials and Glass With An Innovative Ultrasonic Impedance Technique

Longitudinal and shear ultrasonic properties of soft materials are needed to completely characterize the high frequency linear viscoelastic properties of a material. Due to high attenuation, shear properties can only be determined by surface impedance method for soft materials. Until now, few good reliable shear property data are available for soft materials because of the intrinsic difficulties involved in the measurement. An innovative new device and data-analysis system, USMA (ultrasonic soft material analyzer, patent pending), has been successfully developed. The system is used to study the adhesion dynamics between a glass substrate and different soft materials such as elastomers of different base polymers with different carbon blacks, different carbon black concentrations, different mixing conditions and other materials such as hydrogels, tofu, etc. We are able to determine the degree of interfacial contact as function of contacting time, pressure, etc. for these materials. With our innovative approach, we are able to determine accurately ultrasonic shear properties of soft materials, which is a significant contribution towards better understanding of the high frequency viscoelastic properties of these materials.

Ultrasonic Non-destructive Evaluation of Polymer Composites and Adhesive Thin Layer

Regular and defected (tape implanted, pressure excessively applied to create a low-resin content and micro voids due to trapped volatile as result of fast heating cycles) samples of phenolic/fiberglass laminates and unsaturated polyester/fiberglass laminates were evaluated by ultrasonic pulse-echo technique and densiometer. Results base on the double-blind tests clearly demonstrate the power of this simple technique to detect the defected specimens. In order to quantitatively determine the properties of a defect or an insert material or an adhesive layer, we select a simpler substrate material: glass. During the characterization of the glass specimens, we realize that the intrinsic uncertainties in the pulse-echo technique, which could lead to a significant error in the loss tangent value. A systematic approach was developed to improve the measurement. The loss tangents of different glasses are determined at 3.5 MHz and 20 MHz. Thin layers of hydrogels, which are prepared by B. Kim, another graduate student, will be evaluated by placing a thin layer sandwiched between two pieces of thin glasses.

Polystyrene Bead Filled Hydro-gels

Hydrogels have received significant attention because of their exceptional promise in biomechanical applications. Hydrogels of linear copolymers composed of *N*-isopropylacrylamide (NIPAAm) with acrylic acid (AAc), 2-acrylamidoglycolic acid (AAmGAc), and 2-acrylamido-2-methyl-1-propanesulfonic acid (AMPS) are prepared. In order to improve as well as to control the mechanical and diffusion properties of the hydrogels, they will be covalently bonded to polystyrene beads with diameter of 30 nm or less, which are prepared by micro-emulsion polymerization. The mechanical properties at different temperatures and different pH values will be studied by USMA.

Preparation of Nano Polystyrene Beads by Microemulsion Polymerization

The smallest polystyrene particle size that has been prepared in the literature with the method of conventional emulsion polymerization was about 50 nm in diameter. In order to prepare particle size less than 50 nm, we need to use micro-emulsion polymerization. We attempt to develop a recipe to reduce the particle size below 20 nm in diameter. Polystyrene beads will then be mixed with hydrogels of polyacrylic acid-acylamide copolymers. Ultrasonic shear and longitudinal properties of PS beads reinforced hydrogels will be studied as functions of bead concentration and size using USMA.

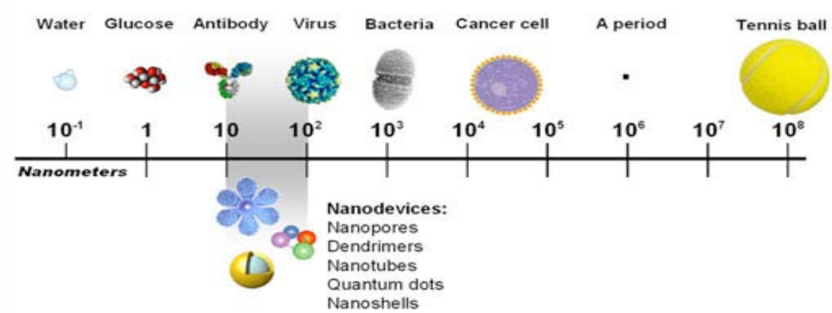
Towards a Tissue-Engineered Tear Secretory Systems: Evaluation of Various Matrix Protein-coated Polymeric Substrata for the Development of a Fluid-Secreting Lacrimal Gland Device

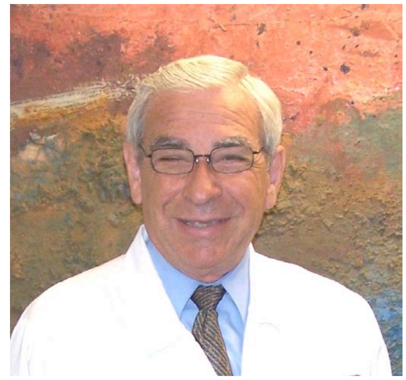
Purified rabbit lacrimal gland cells were cultured on different polymeric substrata: silicone, collagen 1, poly-D,L-lactide-co-glycolide and poly-L-lactic acid (PLLA), and styrene-butadine-styrene block copolymer. The morphological and physiological characteristics of the cells on these polymeric substrata were evaluated. Based on the initial results, PLLA was selected. In order to provide adequate transport properties for small molecules nutrients but also to be able to block higher molecular weight proteins, micro-pores were introduced to the PLLA substrata. The transepithelial resistance and fluid transport of lacrimal epithelial cell monolayers cultured on this polymers are being evaluated.

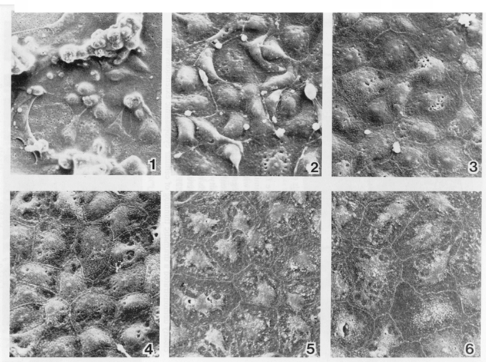
Return to Faculty Research Areas

Edward D. Crandall

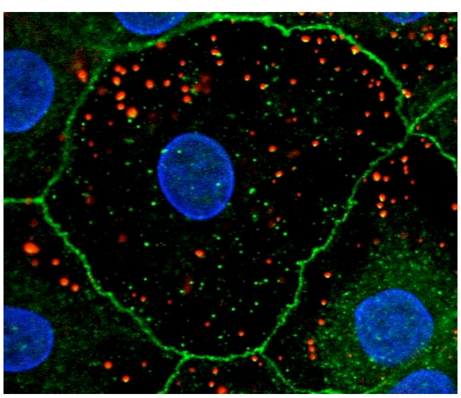
Pulmonary Cell Physiology, Nanoparticles and Lung







Isolated cuboidal alveolar epithelial type II cells are plated on porous filters. Cells in culture from day 1 to day 6 are shown as they spread, become confluent and change phenotype from type II cells to type I cells. We utilize these monolayers to investigate alveolar epithelial cell biology and function, including interactions with nanoparticles.



This confocal photomicrograph shows an alveolar epithelial type I cell monolayer exposed to apical PNP (100 nm, carboxylate-modified) for 24 hours. Cell-cell borders are green, PNP are red and nuclei are blue. PNP are located in cell cytoplasm and not in intercellular junctions or nuclei.

The Will Rogers Institute Pulmonary Research Center has a long history of major contributions in lung cell physiology. Examples of our alveolar epithelial cell monolayer model grown on porous filters are shown. Utilizing this model, we have defined the functional and biological properties of alveolar epithelium. We have recently become interested in determining interactions of nanomaterials with the lung, especially with regard to injury, uptake and trafficking.

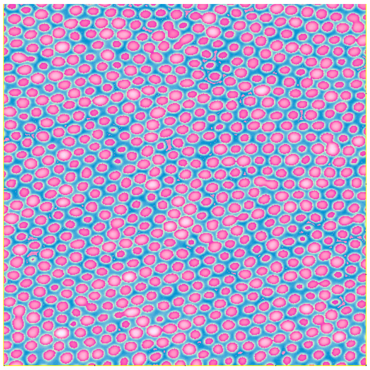
The lung can serve as a portal for entry of nanomaterials (ambient and/or manufactured) into the systemic circulation. Inhaled nanoparticles can be found in heart, bone marrow, blood vessels and other organs, and their most likely route of entry into the circulation is across the epithelia of the lung, especially the alveolar epithelium with its very large surface area and thin barrier thickness. Further knowledge of the mechanisms by which nanoparticles injure, interact with and/or are transported across the alveolar epithelium is thus of considerable importance for understanding health effects related to inhalation of nanoparticles in ambient air.

Interest in nanotechnology has greatly expanded in recent years, driven in part by growth in manufacturing and applications that range widely from fabrication of useful nanoscale circuitry and robotics to biological applications of nanomaterials (particles (see above) having at least one dimension <100 nm) in imaging and transduction at the cellular and molecular levels. Nanoparticles promise to be useful for many biomedicine-related applications, yet their toxicity, trafficking characteristics across cells and specific mechanisms and underlying pathways of uptake into pneumocytes are not well known. We are interested in understanding the influence of nanoparticle (e.g., polystyrene nanoparticles (PNP) or single wall carbon nanotubes) characteristics (e.g., surface charge, size or shape) on trafficking/injury interactions with the air-blood barrier of distal lung (*in vitro* and *in vivo*). Nanoparticle-based drug/gene delivery and regulation of other biological processes are important potential downstream applications of these studies

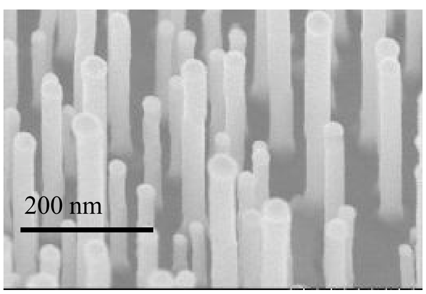
Return to Faculty Research Areas

P. Daniel Dapkus

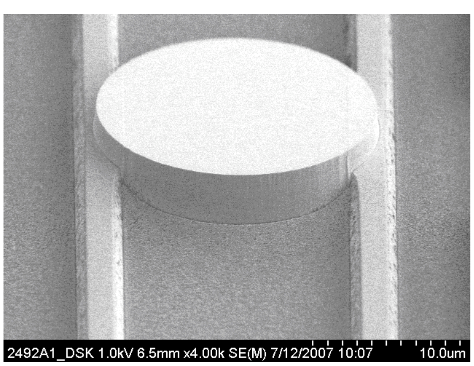
Nanotechnology, Solar Energy, Photonics



Uniform array of InAs quantum dots patterned by using self assembling block copolymers to form a hexagonal close packed array of holes in a hard SiN_x mask for selective area growth of the dots. Subsequent self assembled growth of multiple dot layers on surface with a stress pattern produces multiple layers of dots.



GaAs Nanorods formed by vapor-liquid- solid growth on a (111) GaAs substrate. Other substrates and naorod materials are being used to incorporate these structures into novel devices.



InP / InGaAsP microresonator vertically coupled to single mode buried waveguides using all epitaxial growth techniques and single step, two level, self aligned masking and ICP etching procedures.

In the Compound Semiconductor Laboratory, we are developing novel nanoscale materials structures and device designs that increase the functionality of photonic devices and improve their performance. We are developing engineered quantum dots and nanowires the will improve the performance and lower the cost of solar cells and high efficiency LEDs for solid state lighting. In addition we are developing new processes for the fabrication of microresonator devices that will enable us to fabricate photonic integrated circuits of unprecedented complexity and functionality. Finally engineered quantum dots are being explored as a means to reduced dynamic phase dispersion in the active regions of mode-locked lasers to enable an integrated technology for ultrafast and nonlinear photonic processing.

Nanostructures are engineered by prepatterning the wafer prior to epitaxial growth to control the dimension, density and placement of the nanostructures within the device layers. Novel patterning techniques employing block copolymer lithography and electron bean lithography to pattern strained layers and dielectrics that subsequently control the positioning of the nanostructures by strain or by selective area epitaxy, respectively. Subsequent overgrowth produces two dimensional device structures for incorporation into functioning devices.

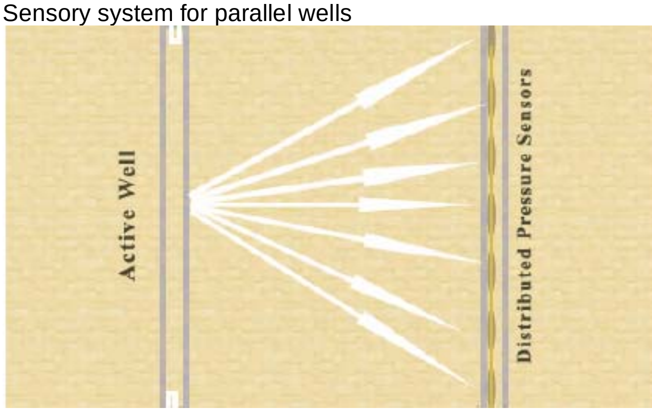
Nanostructures and novel heterojunction designs offer the potential to dramatically improve the efficiency of solar cells and LEDs. We are investigating novel materials processes and materials systems to effect these improvements. We are also investigating novel low cost substrates to dramatically reduce the cost of these devices.

Return to Faculty Research Areas

Iraj Ershaghi

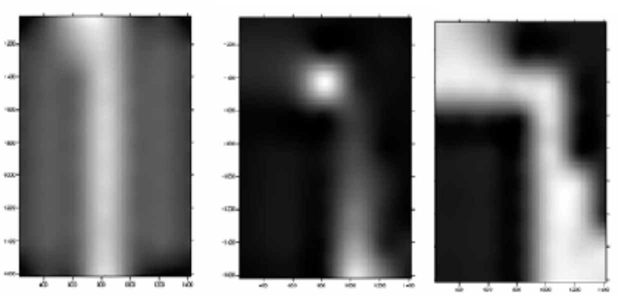
Petroleum Engineering/ Smart Oilfields Technologies

Sensory system for parallel wells



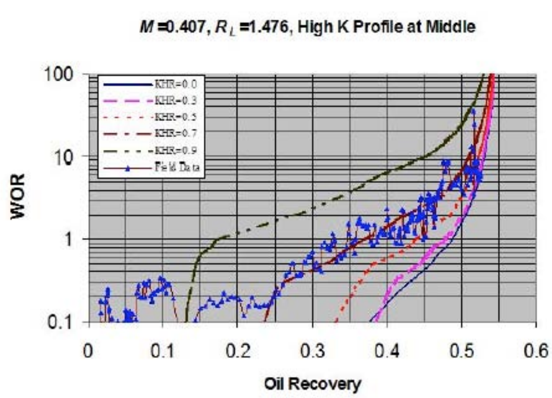
At the Center for Smart Oilfield Technologies we are developing Technologies that can advance the cause of smart resource development and management by infusion of information technologies.

Integration of decision support systems in subsurface, wellbore and surface facilities constitute an important step in enhancing operational reliability, risk avoidance, fault detections and improving resource recovery. Work in progress includes work process modeling and the use of soft computing for risk minimization in decision support systems.



Homogeneous Channel Delta

In the area of oilfield Data mining, an important dimension in smart oilfield management is the automated updating of reservoir models using continuously recorded subsurface and well performance data. Estimation of reservoir parameters such as flow units, rock boundaries and heterogeneities help in identifying compartment in subterranean reservoirs. The dynamic of recorded perturbations in well interferences are analyzed in terms of fluid interferences and the tracking of interfaces.



Diagnostic Plots Results for the Field Case Study.

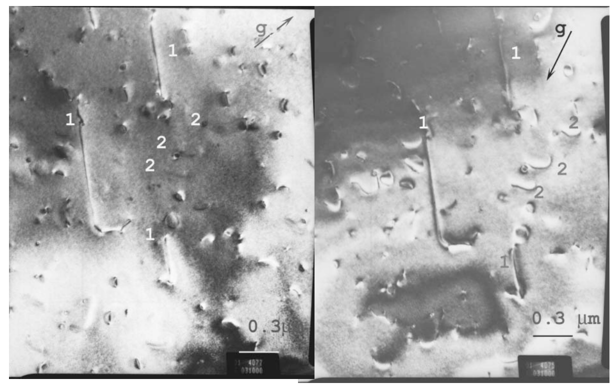
In the area of fracture mapping, we are developing diagnostic techniques to map fracture patterns from performance data. A particular focus is in immiscible processes of water displacing oil where deltas from the behavior of well in a non fractured system are used to detect anomalies associated with the presence of fractures.

Return to Faculty Research Areas

Edward Goo

Phase Transformations and Crystal Defects

Defects in HgCdTe Due to Ion-implantation

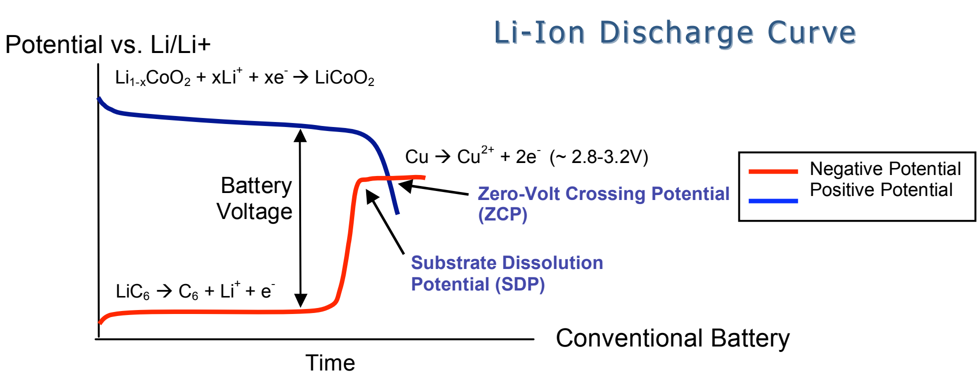


MBE growth of MCT is under Te-rich condition, because, MBE growth under Hg-rich condition results in twin defect formation which can degrade electrical properties [3-4]. The n-type doping of MCT using indium has been accomplished in as-grown MBE. [5]. However, p-type doping is difficult to achieve due to undoped MCT layer grown under Te-rich condition contains high density of Hg vacancies (metallic-site vacancies). A solution is to use ion-implantation of As to produce p-type material. The resulting material even after annealing has a high density of dislocation loops and stacking faults that are being characterized. TEM micrographs shown at right are taken under different imaging conditions are used to characterize the dislocation loops and stacking faults.

Electrode Materials for Li-ion Batteries

Currently Li-ion batteries are unstable in the completely discharged state. This is due to the dissolution of the copper electrode. This is why Li-ion batteries must always be kept charged. For some implantable medical devices this poses a problem. For example in pain reduction devices, the patient may not need operate the device for long periods of time and hence may forgot to charge the device. When the pain recurs, the device will be non-operational due to the failure of the Li-ion battery from being left in the discharged state.

The graph below shows how the Cu dissolution will occur due to the Li compounds in the battery if the cell voltage is allowed to drop to a low voltage.

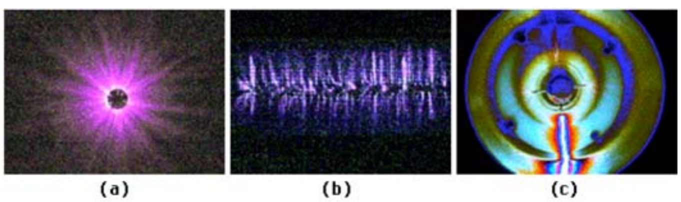


Return to Faculty Research Areas

Martin Gundersen

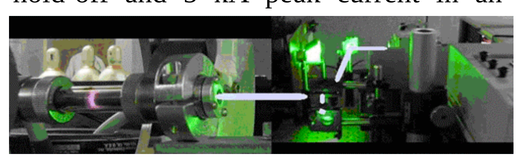
Martin Gundersen conducts research that is *interdisciplinary* with aerospace, biomedical, mechanical, materials science and electrical engineering, medicine, physics, and the entertainment industry. The research group is pictured at the right, and includes students from Chemical Engineering, Materials Science, Electrical Engineeing, Biomedical Engineering, Physics, Biology, and pre-med. Activities include:

Applied Plasma Physics including Transient Plasma Ignition: Transient plasmas, which occur in nanoseconds, are being investigated for *detonation and flame ignition*. For example, recently reductions up to factors of 10 in delays to detonation for pulse detonation engines, and other effects, have been achieved with low energy transient plasma ignition. Validation includes testing at the Naval Postgraduate School Rocket Propulsion Laboratory and Wright-Patterson Air Force Research Laboratory. ("Transient Plasma Ignition," J.B. Liu et.al., IEEE Trans. Plasma Sci. **33**, 2005) A novel physics is involved. The transient plasma produces energetic electrons that *effectively dissociate molecules and generate reactive species* (such as CH and OH), changing the fuel chemistry.



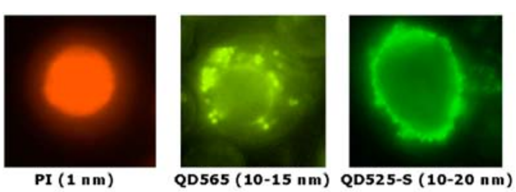
Transient Plasma Ignition: (a,b) End, side views of transient plasma. (c) streamer and arc in combustion chamber.

Pulsed Power: Pulsed power research includes high power switches. A recent paper describes the mini-BLT (Jiang et.al., "Toward Ultra-Compact Pseudospark Switches", Applied Physics Letters **86**, 2005), a finger-sized, high peak power optically-gated switch capable of >25 kV hold-off and 5 kA peak current in an unoptimized system. Interesting physics is associated with it's remarkable super-emissive cathode and electron beam. The BLT is also of interest for EUV generation (Jiang et.al., "Pseudospark Electron Beam as an Excitation Source for Extreme Ultraviolet Generation," *Applied Physics Letters*, **87**, 131501 (2005)).



Laser triggering of MW mini-BLT switch.

Biomedical, Biological, and Medical Applications: We conduct interdisciplinary work with EE, physics, biomedical engineering, medicine, and biology to study the effects of intense pulsed fields on biological cells and tissue. Ultra-short (less than 30 ns), high-field (greater than 1 MV/m) electric pulses induce, for example, increases in cytosolic calcium concentration and translocation of phosphatidylserine in human lymphoblast cells (Vernier et.al., FEBS Letters 572:103-108, 2004, Garon et.al., Int. J. Cancer, March 2007). This research has potential therapeutic applications for cancer and bioengineered devices.

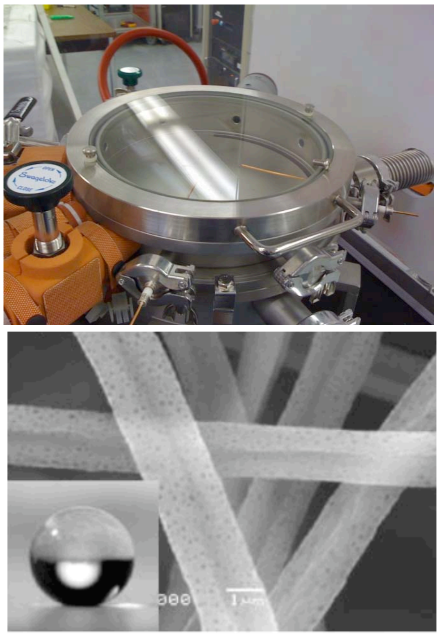


Effects induced internally in various cancer cells by ultra-short high field nanosecond pulses.

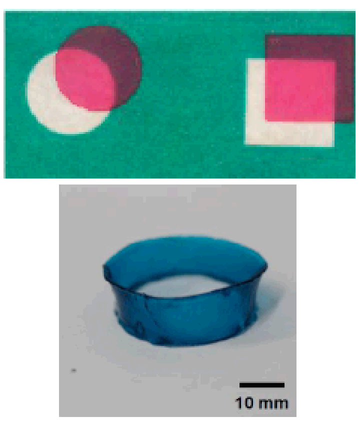
Portrayals in Motion Pictures: Dr. Gundersen is working on improving the depiction of science and engineering in film and television. In one aspect of this work, reported in the New York Times (Aug. 4, 2005), he collaborated with the American Film Institute to conduct workshops for screenwriting for scientists and engineers.

Malancha Gupta

Polymer Coatings, Hydrogels, Surface Science



We use chemical vapor deposition to make thin functional polymeric coatings. Our process is used to coat a wide variety of structures such as membranes, fibers, and wire meshes.



We use patterned templates of paper to fabricate hydrogels composed of cross-linked biopolymers. Our process is used to make topographically and topologically complex shapes and heterogeneous films.

Our lab focuses on fabricating polymer coatings and hydrogels. We use chemical vapor deposition to make thin polymer coatings that can be hydrophobic, hydrophilic, or adhesive. Our process does not require solvents and is therefore environmentally benign. Our coating process is used to change the surface properties of small structures such as microtrenches, nanopores, stents, and probes. We use surface tools such as FTIR, XPS, AFM, and SEM to study the chemical structure and morphology of our polymer coatings. Our coatings have applications in fields as diverse as membrane technology, semiconductor manufacturing, and biomedical engineering.

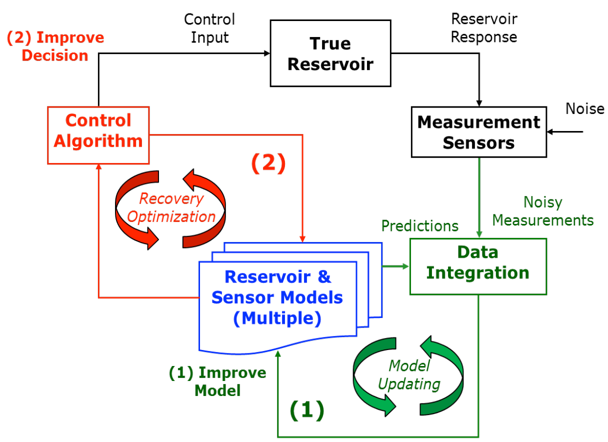
We use patterned templates of paper to fabricate shaped hydrogels composed of biopolymers such as alginic acid and carrageenan. Multivalent cations such as calcium and iron are used as the cross-linking agents. Our hydrogels have applications in tissue engineering and wound dressings. Our fabrication method allows the production of topographically and topologically complex 3D shapes, such as interlocking rings and Möbius strips. We can make magnetically shaped films by using paramagnetic ions like holmium and gadolinium as the cross-linking ions or by suspending ferrite microparticles in the hydrogels. We can also make heterogeneous films of ionotropic hydrogels through the use of multiple templates.

Return to Faculty Research Areas

Behnam Jafarpour

Subsurface Characterization, Energy and Environmental Resources

Subsurface systems pose some of the most challenging characterization and modeling problems in science and engineering with significant environmental, public health, and energy security implications. Significant uncertainty arises from inaccessibility and heterogeneity of geologic formations as well as the complex interactions between fluids and rocks over a wide range of temporal and spatial scales. We are taking a stochastic systems approach for description, characterize, and development of these resources.

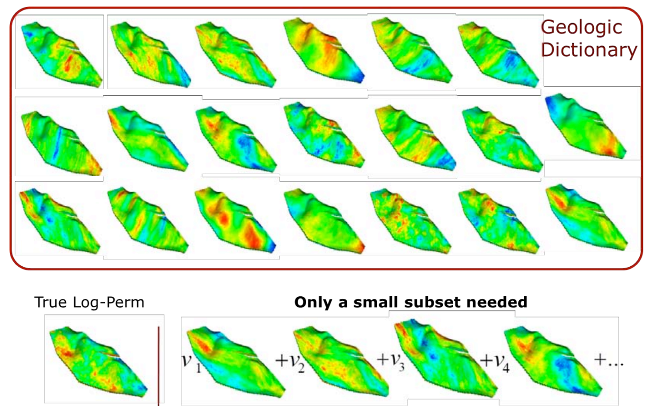


A systems approach for modeling, characterization, and development of subsurface resources.

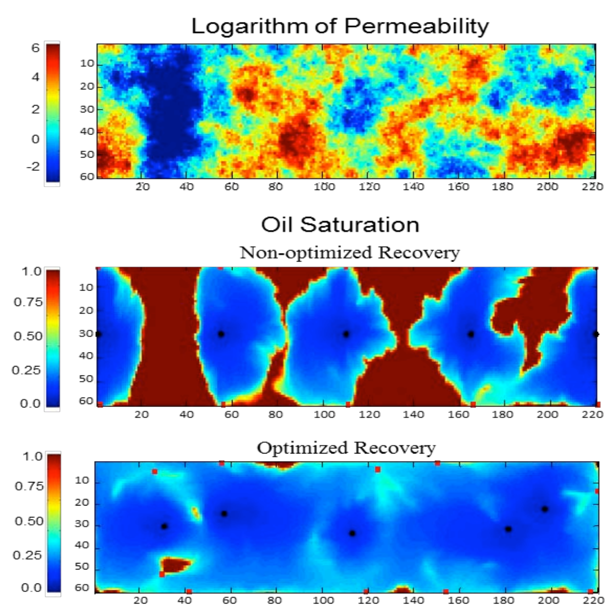
Our research combines advanced computational and mathematical tools of signal processing, estimation, and control theory with insight from geosciences and dynamics of fluid flow in porous media to develop robust and geologically consistent frameworks for solving large-scale subsurface characterization, monitoring, prediction and development optimization problems.

To reliably predict flow and transport processes the connectivity between facies with extreme (high and low) hydraulic properties that create preferential flow paths/barriers must be identified. We are developing feature-based characterization methods to infer complex geologic patterns and their connectivity from dynamic response data.

Predictive models are important tools in forecasting and optimizing the performance of subsurface energy and environmental systems. Another area of research focuses on combining advanced numerical optimization methods with predictive flow and transport models to control and effectively manage the operation and management of energy and environmental resources. Applications that we are currently studying include hydrocarbon reservoirs, enhanced geothermal systems, geologic CO_2 storage and groundwater aquifers.



Sparse geologic dictionaries for subsurface characterization under significant prior uncertainty.



Combined well placement and rate allocation optimization using predictive flow modeling.

Return to Faculty Research Areas

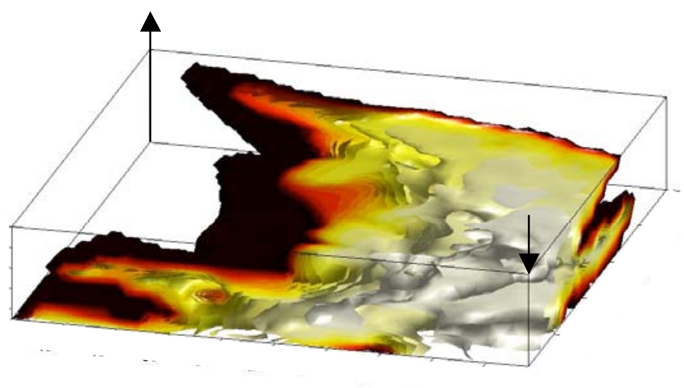
Kristian Jessen

Chemical and Petroleum Engineering

Carbon Sequestration and Enhanced Oil/Gas Recovery

Increasing concentrations of CO_2 in the earth's atmosphere has initiated a wide range of efforts to reduce emissions and to capture and sequester CO_2. Carbon sequestration often refers to a process by which CO_2 is captured from a significant point source, such as a coal-fired power plant, and subsequently injected into a geological formation. Viable candidates for geological sequestration include deep unminable coal beds, depleted oil/gas reservoirs, and deep saline aquifers that are all known to store fluids over significant periods of time.

Design and implementation of CO_2 sequestration projects in underground formations require, in part, a solid understanding of the key physical mechanisms that determine distribution of the injected CO_2 within the target formation. This understanding then forms the basis for model formulation and development of simulation techniques appropriate for resolving the essential physics.



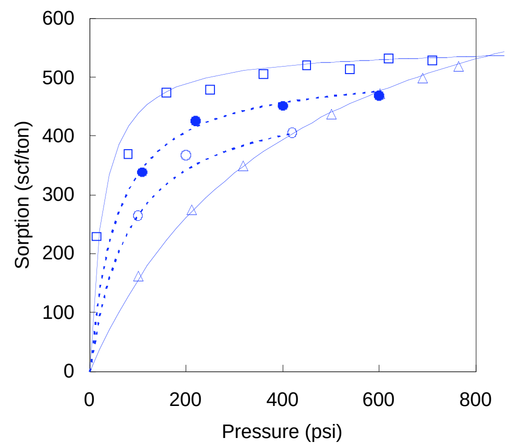
High-resolution compositional simulation of gas injection in a depleted oil reservoir.

In addition, a significant level of uncertainty exists as to the spatial distribution of rock properties. This, in turn, calls for development of simulation tools that are accurate and computationally efficient enough that repeated simulations can be performed to assess uncertainties in predicted movement of the injected CO_2.

In the Carbon Sequestration and EOR research group we investigate and develop accurate physical models that form the basis for development of predictive simulation tools.

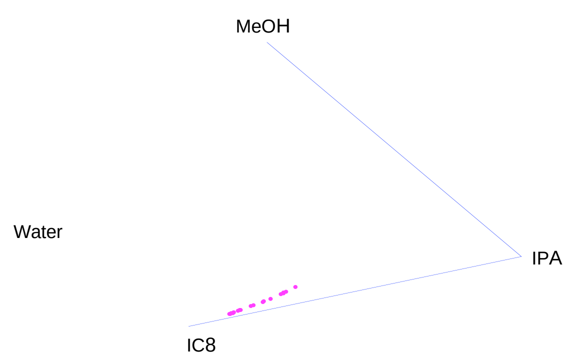
Examples of current research activities include:

- Multicomponent sorption behavior in coalbed methane reservoirs with emphasis on modeling enhanced methane recovery in concert with CO_2 sequestration.



Modeling of sorption hysteresis on coals.

- Dispersive mixing in multicomponent multiphase displacement processes in porous media: Towards an improved accuracy of predictive tools used in the design of enhanced oil/gas recovery and sequestration processes.



Design of an analog fluid system for low-pressure displacement experiments.

Return to Faculty Research Areas

Rajiv K. Kalia
Aiichiro Nakano
Priya Vashishta

Collaboratory for Advanced Computing and Simulations



Nanoscale Science and Engineering is an intellectual endeavor of singular importance that has advanced to a state where complex processes in physical, chemical and materials transformations can finally be understood at the most fundamental level. Profs. Priya Vashishta, Rajiv Kalia, and Aiichiro Nakano at the Collaboratory for Advanced Computing and Simulations (CACS) are involved in research and education at the nano-bio-info interface (Fig. 1). The goals of the CACS are to:

- Follow advances in high performance computing and simulations to study nano-bio systems.
- Establish educational programs across physics, chemistry, biology, chemical engineering and materials science to propel students into careers in emerging areas of nano-bio-info technologies both in academic and industrial settings.

The CACS is using advances in computing technologies (hardware, software, algorithms) — from teraflop to petaflop and beyond — to perform multimillion to billion atom nano-bio simulations. They are developing a scalable parallel and distributed computational framework consisting of methods, algorithms, and integrated software tools for: 1) multi Tera-to-Petascale simulations with quantum-level accuracy; 2) multimillion-to-multibillion atom molecular dynamics (MD) simulations based on density functional theory (DFT) and environment-dependent reactive potentials; 3) mesoscale simulations embedded with classical atomistic and quantum simulations based on DFT; and 4) accelerated molecular dynamics (AMD) coupled with hierarchical atomistic/mesoscopic simulations to reach macroscopic length and time scales. Using this simulation framework, they are studying:

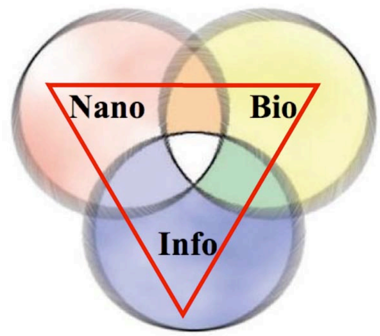


Fig. 1: The CACS research focus.

- Ion transport and translocation of biopolymers such as DNA and RNA through nanometer scale pores and channels in solid-state fluidic devices that underlie “lab-on-a-chip” technology, single nanotube nanofluidic transistors, and solid-state nanopore “microscopy” for molecular structure and high-speed sequencing.

- Stress corrosion cracking (SCC) to understand the atomistic mechanisms underlying SCC and to predict the lifetime beyond which SCC may cause failure.

- Advanced and insensitive nanostructured energetic materials to design new and improved materials and structures with enhanced energy density and reduced sensitivity.

In the educational arena, they have established: A dual-degree curriculum that affords graduate students the opportunity to obtain a Ph.D. in the physical or engineering

Return to Faculty Research Areas

together with an M.S. in computer science with specialization in high-performance computing and simulations (MSCS-HPCS); and an annual series of workshops for undergraduate students and their faculty mentors from underrepresented groups, which provide participants with hands-on experience in parallel computing, including the assembly of a PC cluster from off-the-shelf components, and algorithmic/simulation exercises on it.

CACS Computational and Visualization Facilities

The CACS has 2,048-processor (1,024 AMD Opteron, 768 Intel Xeon, and 128 Apple G5) Linux clusters on Myricom's Myrinet interconnect and gigabit Ethernet switches (Fig. 2). In addition, they have dedicated block access (6 million processor-hours of computing per year through a competitive grant) to the high performance computing facility at USC, which includes the 5,384-processor, 15.8 teraflops Linux cluster. The CACS also has a cluster of Playstation3's for developing multi-core parallel applications

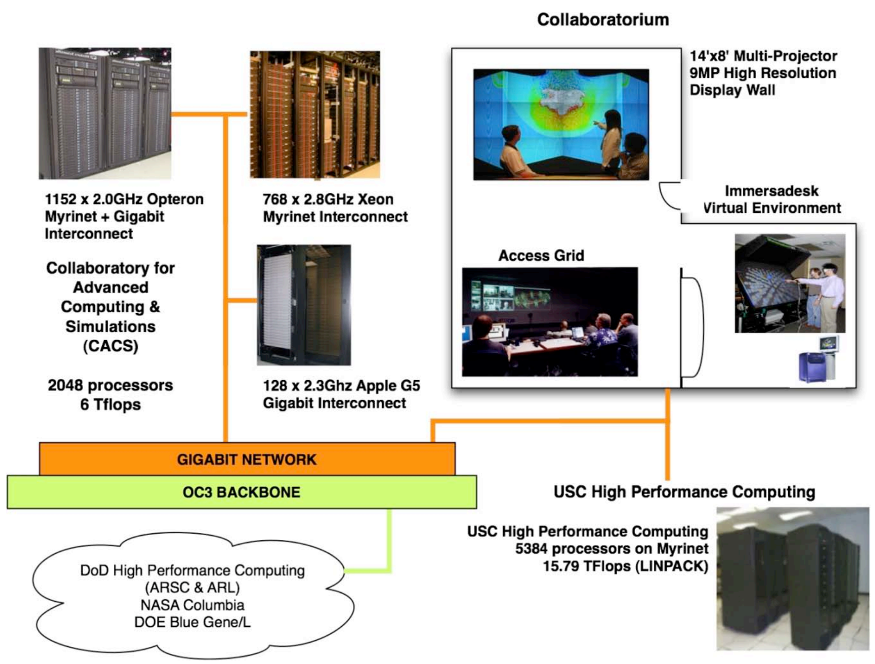


Fig. 2: Parallel computing and visualization facilities at the Collaboratory for Advanced Computing and Simulations (CACS) at the University of Southern California (USC).

Collaborative immersive and inter-active visualization facilities: The CACS also has: (1) a 14'×8' high-resolution tiled display; (2) an immersive and interactive virtual environment, ImmersaDesk; and 3) an Access Grid for remote audio and video collaboration and conferencing.

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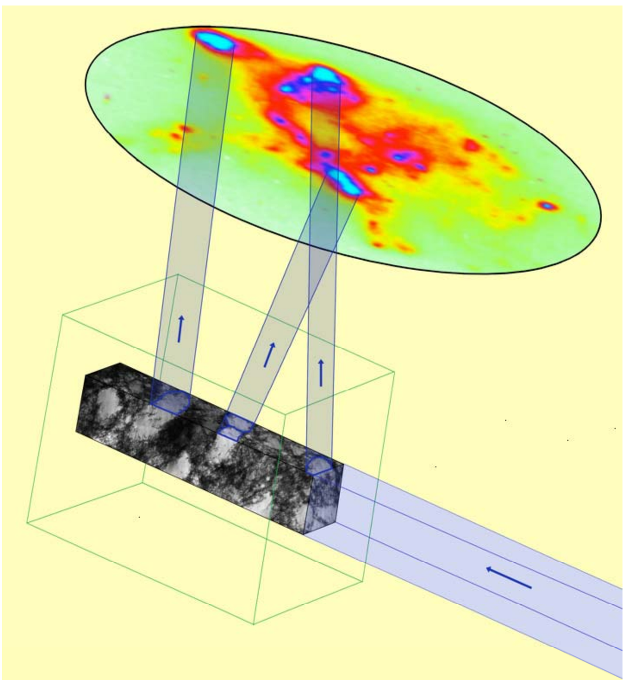
Michael Kassner

Plasticity, Creep, Fracture, Large-Strain Deformation and Fatigue.



Schematic and data from differential-aperture X-ray microscopy done w ith the Advanced Photon Source at Argonne National Laboratory. The incoming X-ray beam is scattered from the sample, shown as TEM photomicrograph, producing the diffraction pattern, shown in false color, on a CCD array.

The Advanced Photon Source at Argonne National Laboratory where the experiments on Long Range Internal Stresses are performed.

Knowing how submicrometer elastic strains distribute themselves within deformed crystalline materials is key to an understanding of numerous important physical phenomena, including the evolution of complex dislocation structures within individual grains, the transport of dislocations through such structures, changes in mechanical properties that occur during reverse loading, and analyses of diffraction line profiles for microstructural studies of these phenomena. Researchers at USC together with Oak Ridge National Laboratory, the National Institute of Standards and Technology, and the Agonnne National Laboratory Advanced Photon Source, recently demonstrated the importance of this type of information of by taking the first direct, spatially resolved, measurements of elastic strains within individual dislocation cells in deformed copper single crystals. Broad distributions of elastic strains were found, which have important implications for theories of dislocation structure evolution, dislocation transport, and the extraction of dislocation parameters from x-ray line profiles. New work is attempting to measure the elastic strains in nanometer-scale dislocation boundaries, with, preliminary success.

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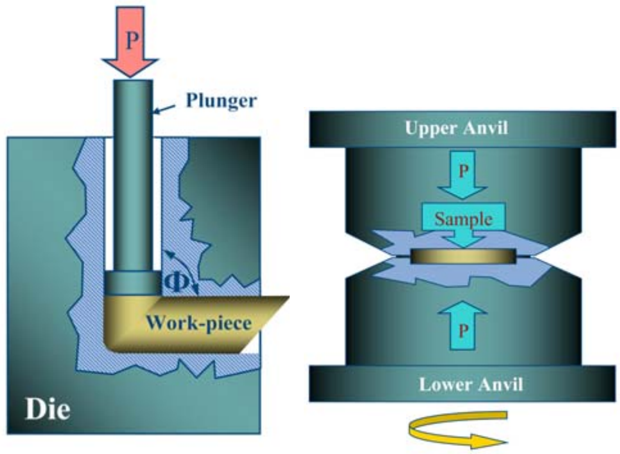
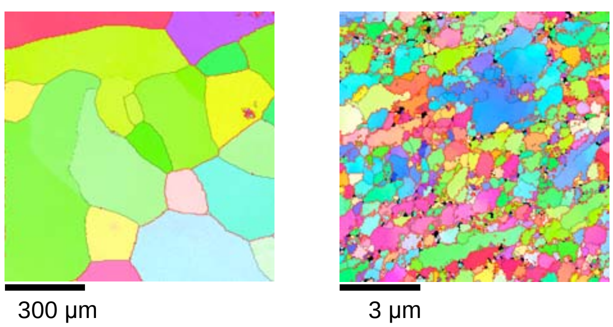
Terence G. Langdon

Nanostructured Materials
Flow Mechanisms in Bulk Solids



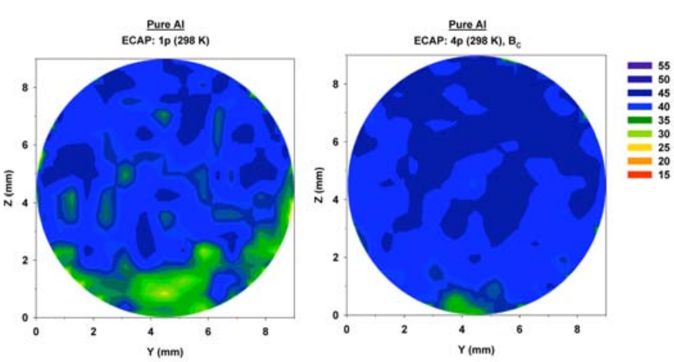
(a) (b)

The principles of (a) ECAP and (b) HPT.



(a) (b)

An example of the effect of processing by ECAP on an Al-1% Mg alloy: (a) in the as-received condition and (b) after 12 passes of ECAP.



(a) (b)

Hardness distributions in pure aluminum after processing by ECAP at room temperature through (a) a single pass and (b) 4 passes.

The processing of bulk nanostructured materials has attracted considerable interest over the last decade. These materials are produced by processing through the application of severe plastic deformation (SPD) in which very high strains are imposed under intense pressures. Several SPD processing methods are now available but the two most important techniques are equal-channel angular pressing (ECAP) and high-pressure torsion (HPT). In ECAP, a material is pressed through a die constrained within a channel that is bent through an abrupt angle. In HPT, a thin disk is subjected to a high pressure and concurrent torsional straining.

Both of these processing methods are capable of producing very significant grain refinement, with the processed grains having sizes typically within the submicrometer or nanometer range. By careful manipulation of the processing conditions, it is also possible to attain good homogeneity within the deformed structures. The reduction in grain size in SPD leads to very high strength at ambient temperatures. Furthermore, if the grains are reasonably stable at elevated temperatures, there is a potential for achieving excellent superplastic forming properties. Thus, materials processed by SPD have the dual advantages of both exceptional strength and excellent formability.

The Mechanical Properties Laboratory at USC pioneered the development and utilization of SPD processing by initiating research in this area in the early 1990's. Currently, we are now recognized at the leading laboratory for this type of research in the United States.

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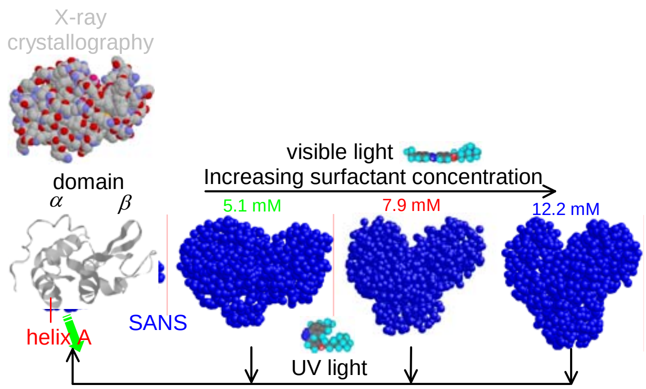
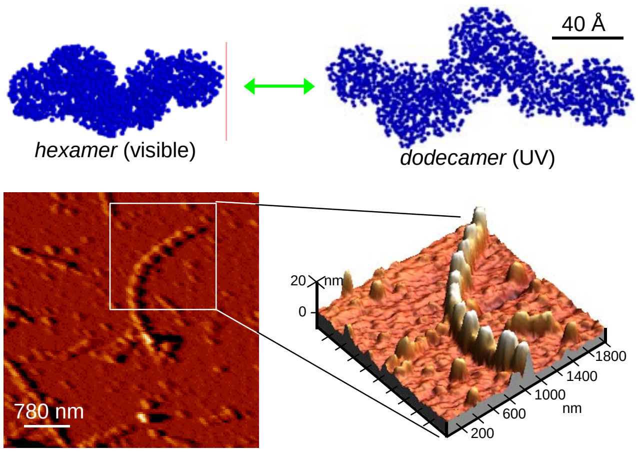
C. Ted Lee

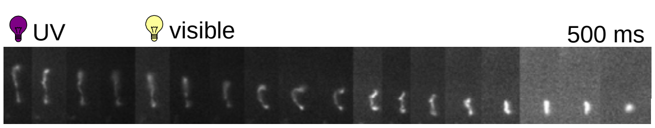
Biomolecular Engineering, Interfacial Phenomena



Lysozyme solution structures from SANS (blue) vs. the crystallographic structure (6LYZ, space-fill and ribbon). Lysozyme unfolding occurs primarily in the α-domain, originating with helix A. The enhanced *flexibility* leads to enzyme *superactivity* (8× more active than the native state).



Control α-chymotrypsin self-association with light revealed through *in vitro* structures of photo-reversible hexamer ↔ dodecamer transitions obtained from shape reconstruction of SANS data, compared to AFM images of amyloid fibrils.



In addition to proteins, the photo-responsive cationic surfactants can interact reversible with anionic DNA. This sequence of images shows photo-induced DNA compaction upon reversible interaction with photo-responsive surfactants, a result of neutralization of the negative charges along the DNA double helix. This technique is currently being utilized to allow photo-enhanced non-viral gene delivery.

Proteins are the workhorses of biology. Beginning as chains of specific combinations of amino acids, proteins fold due to these amino acids having differing degrees of affinity or aversion for water. It is this seemingly-simple folding event, and the resulting shape that the protein adopts in solution, often called the *native state*, which gives rise to a functional protein. However, proteins are not static entities and instead regularly undergo conformational changes to *intermediately-folded states* during the course of activity, particularly upon interaction with other molecules. As a result, precise knowledge of the *structure* of the partially-folded states that form in response to various stimuli, along with the *dynamics* of conformational rearrangements between these states, are required.

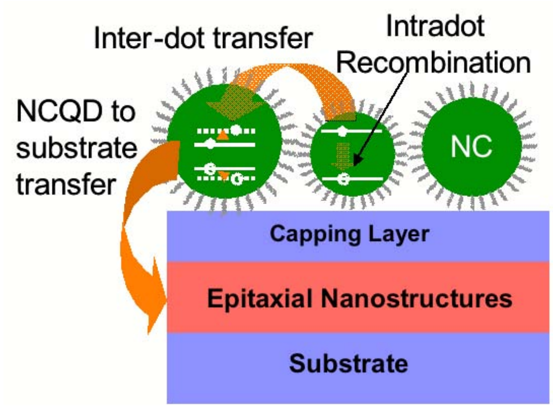
To properly investigate this phenomenon necessitates two complementary approaches: (1) a means to rapidly induce changes in protein folding in a controlled and preferably reversible manner, and (2) a method to determine the conformation of partially-folded proteins at relatively high resolution. To achieve this tandem goal, two novel techniques are utilized in our lab: the interaction of proteins with photoresponsive surfactants to allow photoreversible control of protein folding, and the use of small-angle neutron scattering (SANS) to study the structure of non-native protein conformations in response to photosurfactant and light.

Examples are shown to the left, where SANS "images" of lysozyme reveals a swollen, flexible enzyme with superactivity compared to the native state. Similarly, SANS demonstrates that α-chymotrypsin hexamers with corkscrew shapes wrap around each other to form rope-like dodecamers as the first step in the formation of characteristically twisted amyloid fibers implicated in Alzheimer's disease.

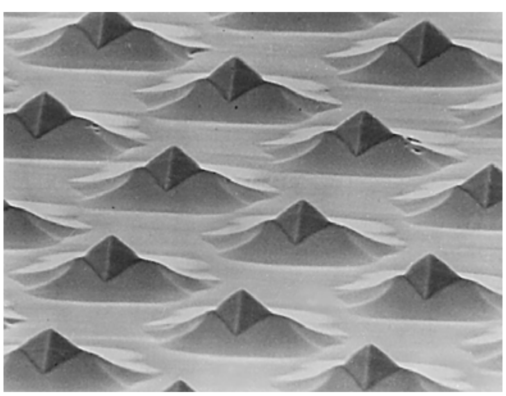
Return to Faculty Research Areas

Anupam Madhukar

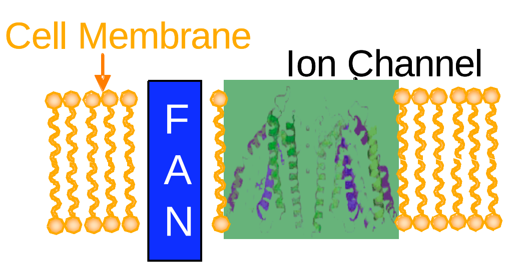
Nanostructure synthesis and structural, optical, & electrical examination; Self-organized nanostructures for radiation detection and solar energy conversion; Abiotic-biotic interfacial phenomena at the nanoscale; Plasma membrane – quantum nanostructure composites for neuronal cell actuation; Live-cell imaging and spectroscopic studies of intracellular biochemical processes.



Hybrid nanocrystal quantum dot (NCQD) and epitaxial nanostructure systems for solar energy conversion and biochemical detection applications



Quantum dot array grown via molecular beam epitaxy (MBE)



Functional abiotic nanosystems (FANs) for probing and actuating cellular processes

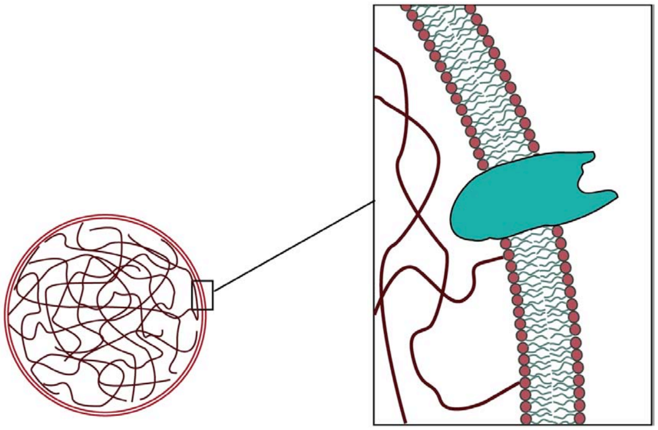
The Madhukar Group (Nanostructure Materials and Devices Laboratory - NMDL) is internationally known for the spawning and development of the field of self-organized semiconductor nanostructures. We carry out multi-disciplinary research with a focus on examining phenomena in novel nanoscale structures and at the abiotic-biotic interface for applications in: computing and communication; conversion of solar photons to power; early detection of biological markers of disease or pathogens in the environment; suppression of immune response to neural prostheses; developing cellular level prostheses we call FANs (functional abiotic nanosystems) for probing and modifying cellular response; and real-time imaging and spectroscopic probing of intra-cellular biochemical processes in live cells under applied stress.

Madhukar holds appointments in Biomedical Engineering, Chemical Engineering, Materials Science, and Physics, and is a member of the Center for Neural Engineering (CNE) and the NSF sponsored Engineering Research Center on Biomimetic Microelectronic Systems (BMES). Students with sound grounding in any science and engineering undergraduate discipline who are dedicated to graduate research in an intellectually challenging, communicative, interactive, and dynamic learning environment are encouraged to find out more about the Madhukar group by visiting our website http://nanostructure.usc.edu and contacting us.

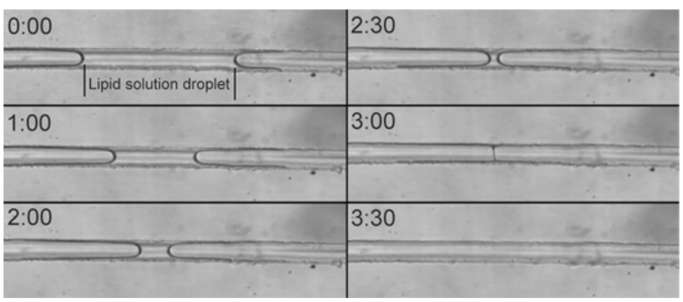
Return to Faculty Research Areas

Noah Malmstadt

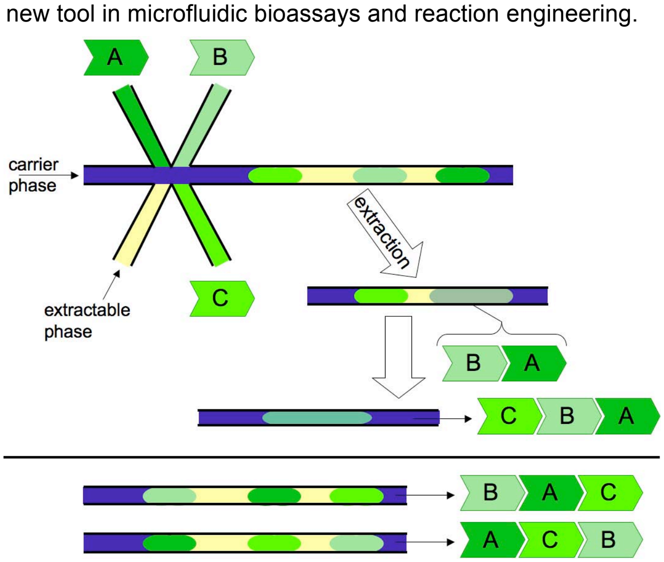
Biomolecular Engineering, Microfluidics



Synthetic, biomimetic membrane-cytoskeleton systems serve as test beds for investigating lipid biophysics and assaying interactions between membrane proteins and ligands.



Solvent extraction in a 100 micron-wide microfluidic channel facilitates the controlled fusion of two flow streams; a valuable new tool in microfluidic bioassays and reaction engineering.



Microfluidic solvent extraction allows for the dynamic reconfiguration of complex reaction schemes in a simple, robust device. This scheme has applications to combinatorial synthesis and high-throughput serial bioassays.

At the Laboratory for Biomimetic Phase Interfaces, we're developing new tools that take advantage of spontaneous phase separation processes to investigate the behavior of biomolecules on the cell surface, to develop new high-throughput and environmentally friendly synthetic reaction systems, and to produce robust, easily deployed microfluidic diagnostic and chemical detection devices.

One of our key areas of focus is the study of nanoscale lipid biophysics. We've constructed "artificial cells" that reproduce the physio-chemical interactions between cell membranes and the cell interior in an entirely abiotic system. We're using high-resolution fluorescence micro-scopy to study how lipids interact with each other on the cell membrane at nanometer scales, and how these interactions change the behavior of membrane proteins. We're also developing screening techniques that use our artificial cells for high-throughput drug development and screening applications.

We're also developing new microfluidic control technologies for robust, easy-to-implement devices. Our devices are based on multiphase flows, in which synthetic and analytical reactions are performed in microreactor droplets. To control the contents of these droplets, we use a fully automated, material-mediated solvent extraction technology. An immiscible phase separates the droplets, and to facilitate droplet mixing, this phase is selectively extracted from the flow stream. This technology has applications in nanoparticle fabrication, environmentally friendly chemical synthesis, combinatorial chemistry for drug development, and high-throughput bioassays for diagnosis and chemical detection.

Return to Faculty Research Areas

Florian Mansfeld

Electrochemistry,
Corrosion Science and Technology,
Batteries and Fuel Cells

What's New at CEEL ?

Prof. Florian Mansfeld, Director of the Corrosion and Environmental Effects Laboratory (CEEL) at USC, and Yuelong Huang, a Ph. D. student at CEEL, have completed the first phase of an extensive study of the corrosion resistance of the Al alloy 6061 that has been anodized and sealed using different novel anodizing baths and sealing treatments developed by Dr. Hong Shih, a CEEL alumnus, who is Technical Director of Etch Products at Lam Research Corp. that is funding this project at CEEL.

Using electrochemical impedance spectroscopy (EIS), which is a non-destructive technique, it was found that the protective properties of the anodized layers prepared by three different processes did not change during exposure to 3.5 % NaCl – a very corrosive solution. One set of samples was exposed for 365 days without any changes of the oxide properties.

In a MURI project funded by AFOSR Aswin Manohar, a Ph. D. student at CEEL, is studying the performance of microbial fuel cells (MFC) using a suite of different advanced electrochemical techniques including EIS to evaluate various factors that can determine the power output of a MFC.

In a MFC bacteria such as *Shewanella oneidensis* oxidize the fuel such as lactate at the anode, while oxygen is being reduced at the cathode. While the power output of MFCs is quite low at present, their advantage is that bacteria can oxidize a large number of different inexpensive fuels and that very expensive alloy catalyst electrodes are not needed. The anode and cathode in the MFCs under investigation consist of graphite felts which are plated with Pt particles at the cathode to enhance its catalytic activity. In order to increase the active area of the anode, stainless balls or graphite granules have been placed into the anode compartment ("packed bed electrode").

Artin Petrossians is applying cyclic voltammetry to deposit Pt-Ir nanowires that can be used as electrodes in the retinal prosthesis project funded by the Biomimetic ERC at USC.

Thomas Valdez, a part-time Ph. D, student, works at JPL in Pasadena, CA on the development of a new generation of fuel cells for outer space exploration.

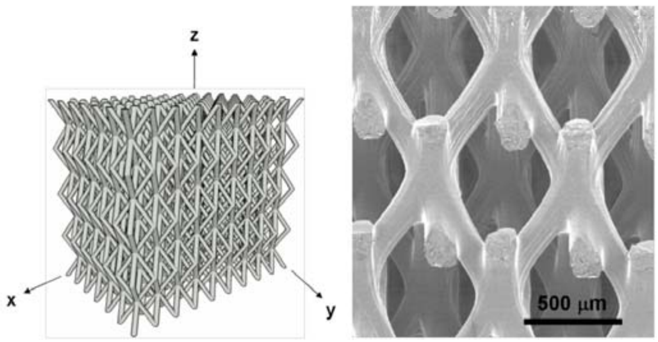
Yi Shi, a Ph. D. student, is studying different modifications of bacterial batteries using electrochemical techniques.

Dr. Zhen He, a post-doctoral fellow, is conducting research dealing with the development of microbial fuel cells for oilfield applications. He is assisted by Yuelong Huang. Prof. Mansfeld is the PI of this project that is funded by the Center for Smart Oilfield Technologies (CiSoft) of USC and Chevron Center of Excellence for Research and Academic Training. Dr. He is also working on ammonia-based MFCs and phototrophic MFCs.

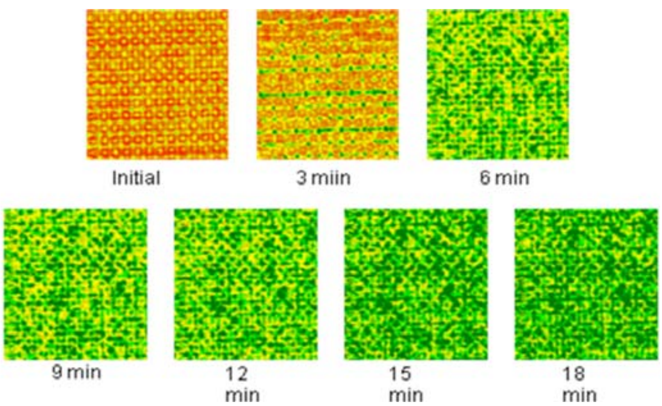
Return to Faculty Research Areas

Steve Nutt

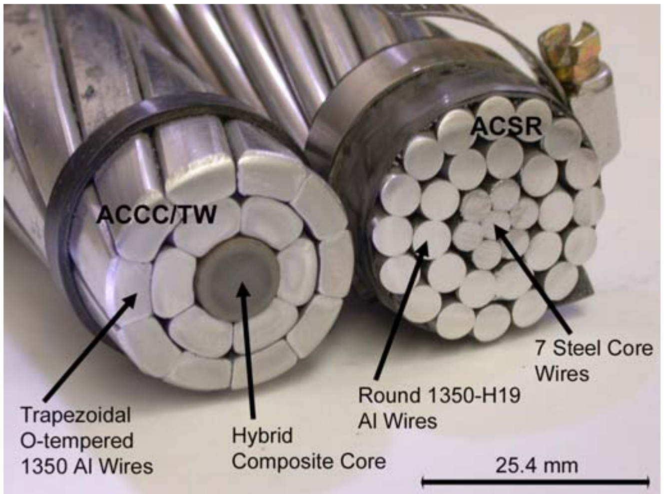
Materials Engineering, Composites



Microtruss structure four unit cells in height, and SEM image of model structure produced from self-propagating photopolymer waveguides.



Ultrasound images monitoring flow front in situ during Impregnation of carbon-fiber low-pressure prepreg laminate.



Composite power line and conventional power line. The conductor consists of a structural core wrapped with strands of Al wire. In the new design at left, a hybrid glass-carbon composite core replaces a stranded steel cable core at right. The composite conductor features low sag at high temperatures, and thus greater ampacity.

Within the Gill Foundation Composites Center, we are developing lightweight composite materials and structures for aerospace, energy, and infrastructure applications. The activities include analysis of new manufacturing methods, measurements of mechanical properties and damage mechanisms, and computer simulations.

In one of our projects, we are working with local industry to develop a composite-reinforced power line for more efficient energy distribution. The power lines can carry more current with less sag and lower line losses than conventional overhead conductors, saving energy while simultaneously reducing the cost of expanding distribution capacity. Within the Center, we are conducting accelerated aging experiments to determine degradation mechanisms that limit long-term durability.

We are also engaged in research to develop new composite materials and methods for producing composites. In one project, we are developing new core materials for sandwich structures. These ultra-lightweight cellular materials include fiber-reinforced foams and micro-truss materials that may outperform honeycombs. In a related project we are undertaking processing science to understand the effects of process parameters on impregnation of fiber fabrics. This process is used to make a new kind of low-pressure prepreg that may one day replace autoclave processing, a costly method commonly used in today's aerospace industry to produce high-performance laminates.

The Center presently includes 15 graduate students, 3 postdoctoral fellows, a visiting professor, 3 undergraduates, and a laboratory manager.

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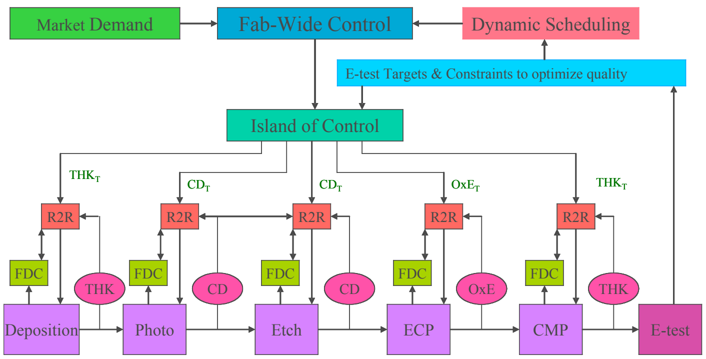
S. Joe Qin

Process Control, Monitoring, and Optimization



Hierarchical, multi-step control and fault monitoring applied to a semiconductor manufacturing fab. Each processing step is optimized in real time for a specific process condition to make high quality products and minimize waste.

Due to increased requirements on process efficiency, product quality, and environmental regulations in process operations, advanced process control offers enabling solutions to these industrial challenges. The emergence of model predictive control, optimization, and process monitoring provides a tremendous opportunity to improve process efficiency and optimality. Our specific research areas include

- Model Predictive Control and Performance Optimization
- Modeling and System Identification
- Process Monitoring and Fault Diagnosis
- Semiconductor, Chemical, Pulp and Paper, and Oilfield Management Processes

Model predictive control (MPC) is by far the most effective advanced control strategy in process industries. Recent academic research has built the connection between MPC and the linear quadratic regulation and state estimation problem.

Remaining challenges lie in the area of MPC performance optimization and fault tolerant control. Our objective is to develop Performance assessment and diagnosis methods for underperforming subsystems, on-line model validation, and disturbance change detection. We are interested in applying MPC to nontraditional areas such as semiconductor manufacturing and oilfield development.

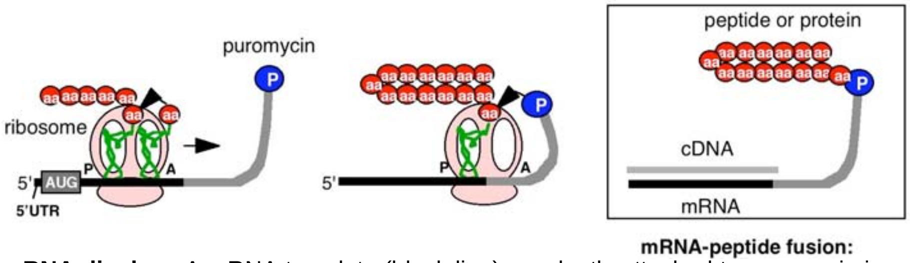
System identification for multivariable processes is very important for applying model predictive control and process monitoring. Current industrial practice almost exclusively relies on system identification to derive the process model. Challenging problems include closed-loop system identification, multivariable structure determination, and modeling of unmeasured dynamic disturbances. Our objective is to develop new methods based on subspace identification methods, partial least squares and advanced statistical methods to overcome these problems.

Process monitoring and fault diagnosis play a significant role in safe process operation and control. We make use of principal component analysis, partial least squares, dynamic models, and wavelet theory to detect abnormal process conditions and sensor faults. The objective and challenge are to identify the root cause of any abnormal situations that could happen in a process.

Return to Faculty Research Areas

Richard W. Roberts

Peptide and Protein Design
Biomolecular Engineering, Signal Transduction, Evolution



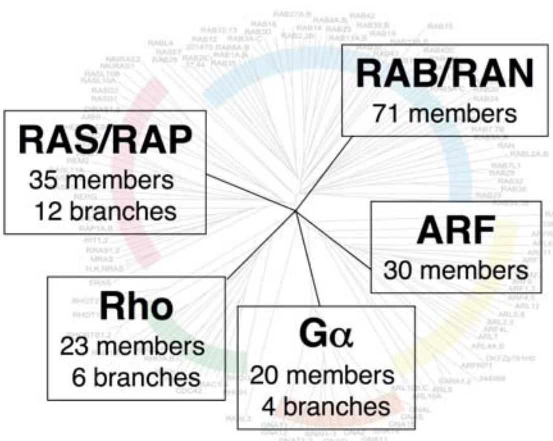
mRNA display. A mRNA template (black line) covalently attached to puromycin is used to program an *in vitro* translation reaction. After protein synthesis, the puromycin enters the ribosome *in cis* to form a covalent mRNA-protein fusion (3).

The Roberts lab works on peptide and protein design and the origin of the ribosome. We use **mRNA display**, to enable polypeptide design (see mRNA display figure at left) (*3*). Using mRNA display, we can create and sieve more than 100 trillion independent peptide or protein sequences using *in vitro* selection and directed evolution experiments. Our projects are:

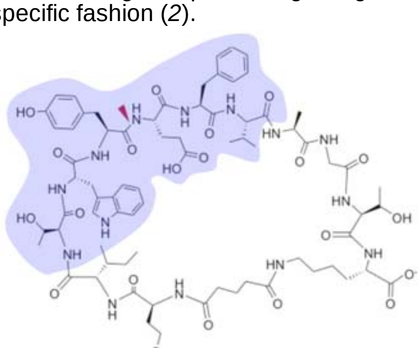
1. **Designing peptide drugs that target protein surfaces**. We have designed peptides that extend lifespan in fruit flies (*2*) and cyclic peptides that bind signaling proteins with antibody-like affinity (*1*) (bottom figure). Our current focus is designing molecules that target G protein mediated signal transduction (*4*) (middle diagram). We are also interested in expanding the genetic code, merging the power of display selections with the flexibility of combinatorial chemistry (*4*). Our long-term goal is to develop new, cell-permeable modulators of protein-protein interactions as rational therapies for cancer, aging, and other human disease states.

2. **Designing intrabodies.** We have also been designing disulfide-free proteins that can be used as high-affinity intrabodies in live cells (*5*). These proteins are based on the human fibronectin 10FnIII scaffold. Our long-term goals are developing i) phospho-specific proteins that recognize covalent modifications, ii) proteins to assist live cell imaging, and iii) proteins that enable testing therapeutic hypotheses about important diseases such as HIV-AIDS and SARS.

3. **Exploring the molecular origin of the ribosome.** This project explores our hypothesis that the modern ribosome is a molecular fossil of the primordial RNA replicase. Our long-term goal is to address one of the major issues in the evolution of life on earth, the transition from a hypothetical RNA organism to the Last Universal Common Ancestor (LCA).



The G protein Superfamily. We are developing molecules that target G protein signaling in a state- and class-specific fashion (*2*).



cycGiBP
(K_d = 2 nM)

A cyclic peptide designed using mRNA display (*1*).

References
1. Millward et al., *ACS Chem. Biol.* **2**, 625-634 (2007).
2. Ja et al., *Nature Chem. Bio.* **3**, 415-419 (2007).
3. Takahashi et al., *TiBS* **28**, 159-165 (2003).
4. Ja et al., *TiBS* **30**, 318-324 (2005).
5. Olson et al., *Prot. Sci.* **16**, 476-484 (2007).

http://mrnadisplay.usc.edu/
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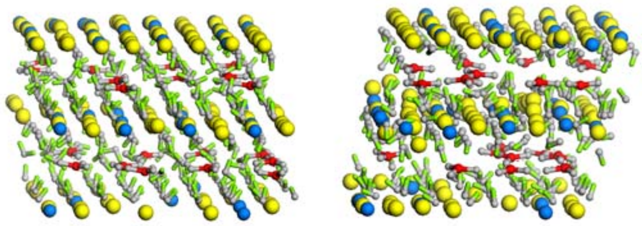
Return to Faculty Research Areas

Muhammad Sahimi

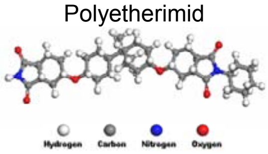
Nano- and Large-Scale Porous Media, Biological Molecules in Confined Environments, Atomistic and Large-Scale Simulations

Layered Double Hydroxides

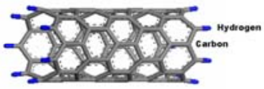


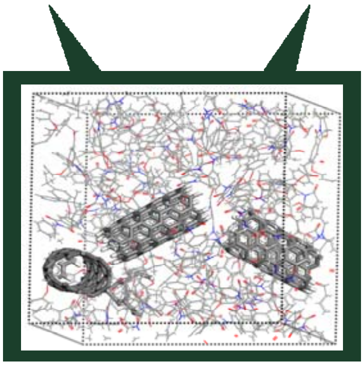
At low temperature | At high temperature

Polyetherimid

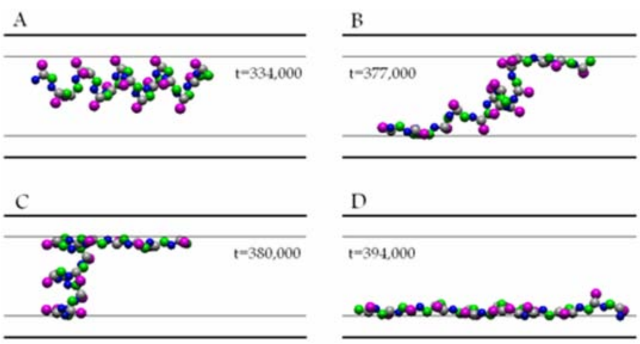


Carbon nanotube



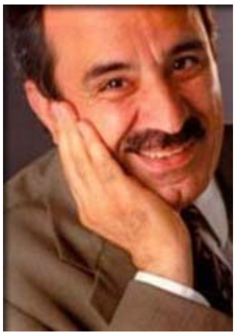


Polymer Composite



Protein folding in a nanopore

One area of our research focus is on nanoporous materials, and in particular several types of membranes for separation processes, and thin films.



The experimental work on membranes is carried out in the Laboratory for Membrane Separation Processes and Reaction Engineering, jointly run with Professor T. T.Tsotsis. Atomistic modeling of these and other materials, such as composite solids consisting of a polymeric matrix in which carbon or SiC nanotubes have been inserted, are also being developed using realistic force fields, and molecular dynamics simulations. Areas of research include transport of multicomponent mixtures, and mechanical properties of the materials. Also studied are molecular simulations of formation of nanoparticles.

A second area of focus is large-scale porous media, and in particular landfills and oil reservoirs. We are developing new computational strategies for analyzing the experimental data for such porous media, developing detailed computational models based on the data, upscaling the models to coarsened levels suitable for simulations, and studying various phenomena in such models, including diffusion, reaction, and multiphase flows. Tools of our studies are Markov analysis, the Genetic Algorithm and simulated annealing, artificial neural networks, and large-scale and massively-parallel numerical simulations. In a separate project, we are studying propagation of acoustic and elastic waves in large-scale porous media (oil reservoirs, rock), as well as heterogeneous solids, and their implications for modeling of such media. Tools of our study are renormalization group methods and large-scale computations.

The third area of research is concerned with the behavior of biological molecules in confined environments, such as cells and nanopores. We are studying the stability and transport of proteins in nanopores, DNA translocation, and development of novel methods for detecting the protein- and RNA-coding segments of DNA molecules. Tools of our study are molecular dynamics and Monte Carlo simulations, analytical analysis, and computation of the Shanon entropy.

Return to Faculty Research Areas

Katherine Shing

Thermodynamics, Molecular Simulation, Supercritical Fluids

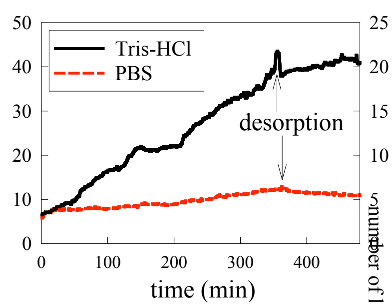


Fig.1. IgG adsorption amount and estimated layers as a function of time at 0.1mg/ml bulk concentration in Tris-HCl and in PBS on ZnSe surface

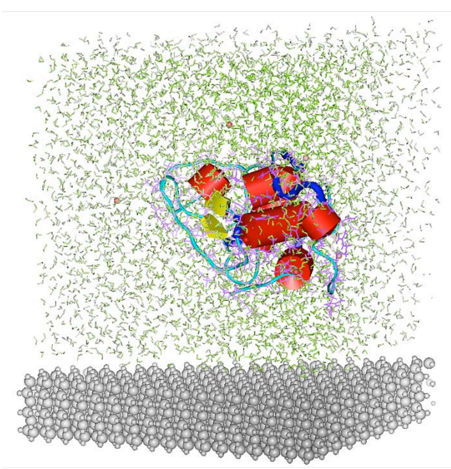


Fig.2. Snapshot of lysozyme on H-Si surface in the explicit water environment together with counter ions

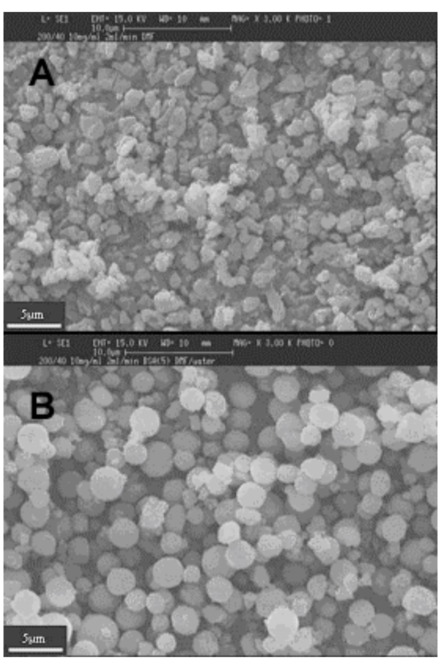


Fig. 3. The effect of albumin addition on particle morphology; A: pure drug (ipratropium bromide) particles, B: drug particles with 5% albumin

We use experimental and simulation methods to study the behavior of molecules and particles in fluids or at interfaces.

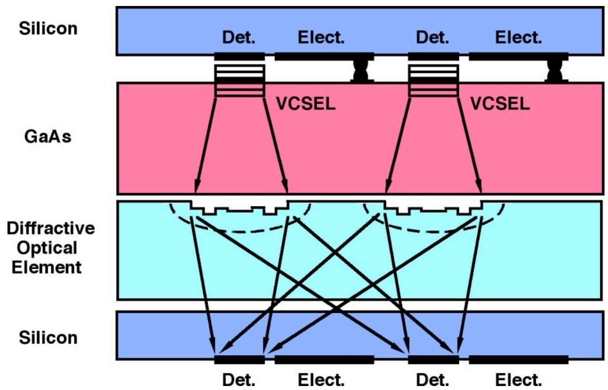
One study combines Fourier-transformed-Infrared Spectroscopy (FTIR) and Molecular Dynamics (MD) simulation to study protein adsorbed on solid surfaces. The FTIR studies reveal the adsorption kinetics as well as the protein secondary structures during adsorption. For example, we show that the adsorption of certain proteins (such as IgG) on certain surfaces is heavily influenced by the type of buffer used. (Fig.1). The MD simulations on the other hand, probe the protein conformations, conformational changes Fig.2), as well as the crucial roles of solvent molecules, buffers, ions and additives such as surfactants.

Another study in our lab examines the production of drug particles for inhalation therapy. The key objectives are to prepare particles in the respirable size range (1-5 microns) with consistent aerodynamic properties. We use a CO_2 based supercritical ant-solvent process which offers a flexible range of operating conditions and solvent choice. By optimizing the operating conditions and additives (such as BSA), particles size and shape can be significantly enhanced. (Fig.3).

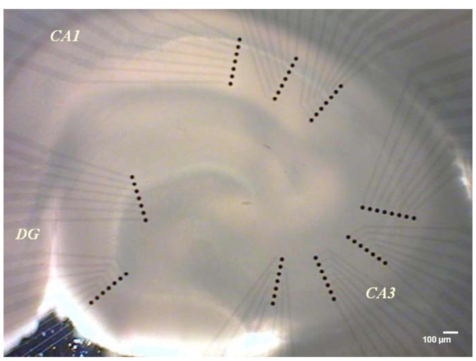
Return to Faculty Research Areas

Armand R. Tanguay, Jr.

Optical Materials and Devices; Retinal and Cortical Prostheses



Schematic diagram of a multilayer hybrid electronic/photonic computation/interconnection element, with vertical cavity surface emitting laser and diffractive optical element arrays.



Trisynaptic pathway conformal multielectrode array proximity coupled to an acute rat hippocampal slice, with electrodes positioned accurately with respect to the cytoarchitecture of the dentate gyrus (DG), as well as the CA3 and CA1 regions.

Original images in color and grey scale (left), pixellated at 25 x 25 (center), and then 33% Gaussian blurred (right), showing the use of visual psychophysics to provide design contraints for the intraocular camera for retinal prostheses.

Research within the Optical Materials and Devices Laboratory includes the crystal growth and characterization of optical and optoelectronic materials; dielectric and optical thin film physics; thin film deposition technology and characterization; device processing by ion beam milling and etching techniques; electronic/ photonic packaging including multichip module integration by flip-chip bonding; physical optics; the physics and technology of electrooptic, optoelectronic, and integrated optical devices; photonic implementations of neural networks; smart cameras (including adaptive nonlinear dynamic range compression and color constancy); surgically-implantable intraocular cameras and multielectrode arrays for retinal prostheses; immersive panoramic cameras; chaos in neural networks; 2-D and 3-D conformal multielectrode neural probes and neural unit array prostheses for the brain; hybrid biological/electronic/photonic computational modules; and the fundamental and technological limitations of optical information processing and computing.

Current research programs within OMDL are highly interdisciplinary in nature, and include the development of hybrid electronic/photonic multichip modules for vision applications; the design, fabrication, and testing of an intraocular camera to be used in conjunction with advanced conformal multielectrode arrays to form a retinal prosthesis for blindness induced by retinitis pigmentosa and macular degeneration; the use of human psychophysical techniques to develop optimal image acquisition and stimulation protocols for retinal prosthetic devices with limited numbers of microstimulator electrodes; the study of lateral brightness and chromatic adaptation in the human visual system; and the search for the fundamental origins of layering throughout the human visual and cortical systems.

Return to Faculty Research Areas

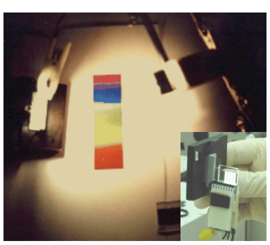
Mark Thompson

Materials Science, Organic Electronics

Chemists have focused the majority of their attention on synthesizing and studying compounds on a molecular level. The end result of this work is the ability control both molecular structure and properties very efficiently. The major thrust of my research at USC is aimed at extending the control chemists have developed for molecular species to solid materials. We have focused on molecular polymeric materials for optical studies in recent years and have recently extended out interests to include tailoring the properties of the nanomaterials as well. In the material given below I will highlight our recent work in the areas of electroluminescence in organic materials, photochemical

Organic LEDs

Considerable research is currently focused on the development of new light emitting device technologies. One technology that shows promise are organic light emitting devices (OLEDs). These devices are built from a variety of different molecular and polymeric materials, which serve as electron and hole carriers, sites of recombination and luminescent zones. Our research on OLEDs addresses a number of issues, including the mechanism of electroluminescence, the stability of and lifetimes of OLEDs, and the identification of new materials and device architectures for OLEDs. Our work color tuning these devices, has led to a deep understanding of the mechanism of electroluminescence. With the use of both fluorescent and phosphorescent dopants we have tuned the OLED color from blue to red with high efficiency. Our best devices emit with nearly 100% efficiency (photons/electrons), exceeding the best efficiencies reported for conventional LEDs. We have recently turned our attention to the study of white light emitting devices, with applications for general illumination.



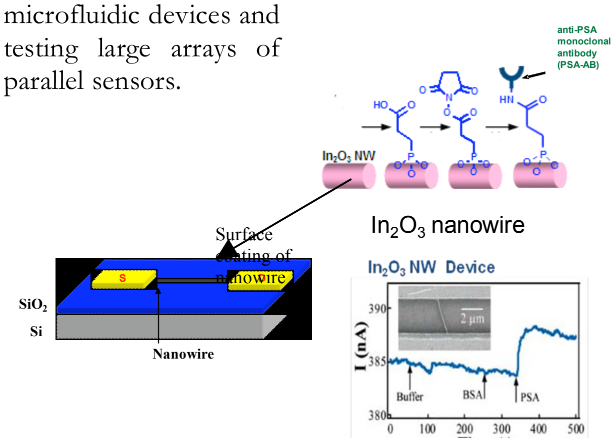
White emissive OLED

Photochemical Energy Conversion

We are also interested in the use of organic and organometallic materials for studying photochemical energy conversion. This can be thought of as a microscopic reverse of the electroluminescence process, but the materials demands for achieving high efficiency solar energy conversion are very different. We are working to develop novel materials sets that are tailored to the photochemical energy conversion process. There is a great deal of interest in the scientific community in the development of renewable energy sources. Solar energy has the potential to replace some of our dependence on fossil fuels, but only if the solar panels can be made very inexpensively and have reasonable to high efficiencies. Organic solar cells have this potential.

Nanobiosensors

Our research focuses on the development of sensors constructed using nanomaterials such as carbon nanotubes and indium oxide nanowires. The most promising nanobiosensors are the those based the electrocnic detection of the target molecule such as field effect transistor nanosensors (FET). These devices are still in the early stages of development but have made impressive progress over the past 5 years. Each single nanobiosensor is capable of identifying the specific biomarker for which it was designed, at biologically relevant levels. We are currently working to develop novel methods for fabrication nanobiosenosrs, integrating them with microfluidic devices and testing large arrays of parallel sensors.

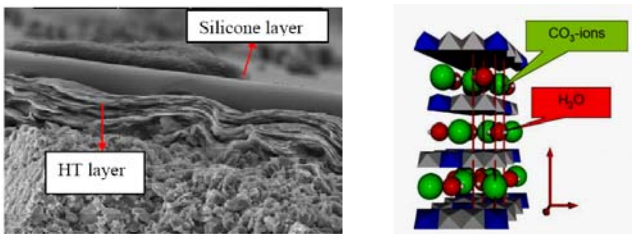


In_2O_3 based bionanosensor for PSA

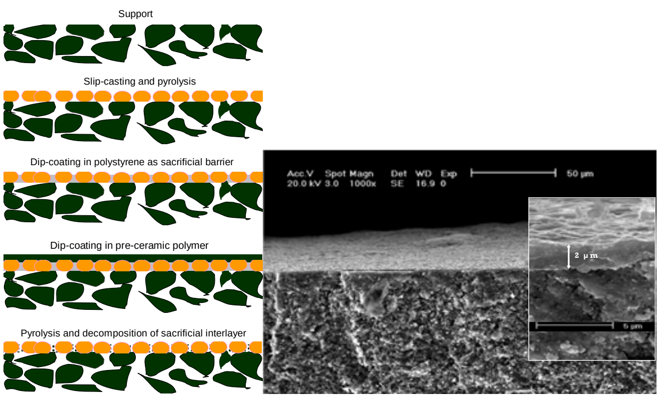
Return to Faculty Research Areas

Theodore T. Tsotsis

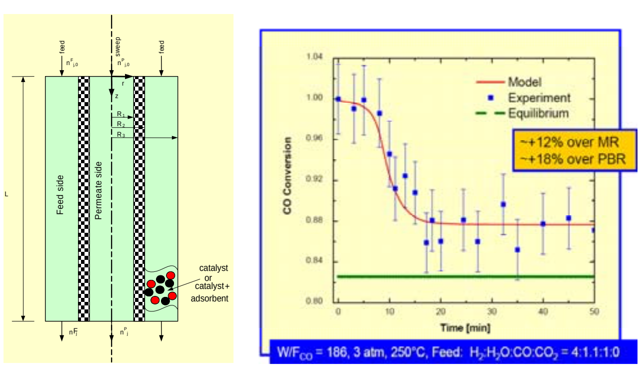
Membrane Separation Processes, Reaction Engineering



Left, the cross-section of a silicone-coated HT membrane (Magnification × 5K); right the HT structure.



Left, the new sacrificial interlayer-based technique developed for preparing SiC membranes; right the SEM picture of a SiC membrane.



Left, a schematic of the HAMR system; right CO conversion for the WGS reaction with the conventional packed bed, and the HAMR. Also, shown are the predictions using the model developed for the HAMR.

In the Laboratory for Membrane Separation Processes and Reaction Engineering, we are developing new membranes for both conventional and reactive separation processes.

A key focus area is the study of materials, which are potentially good candidates for preparing novel membranes for use in the separation of H_2 and CO_2 from their mixtures. We have developed SiC, carbon molecular sieve, hydrotalcite (HT), and mixed-matrix membranes using techniques such as chemical vapor deposition, dip-coating, electrodeposition, and pyrolysis. These membranes are thermally and mechanically stable.

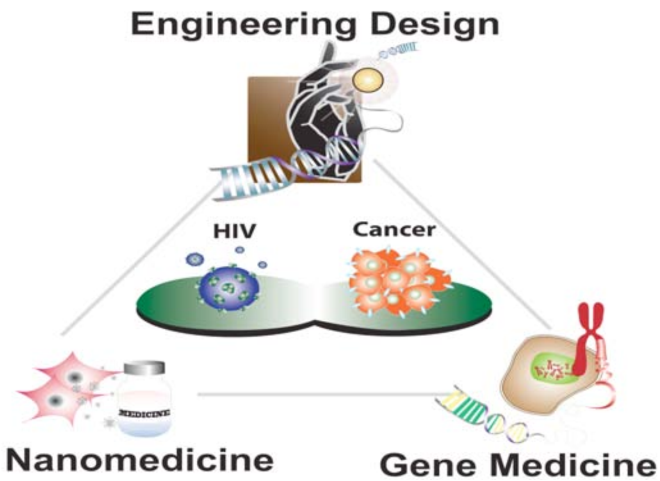
In particular, we are developing SiC membranes using techniques such as chemical vapor deposition and the pyrolysis of pre-ceramic polymers. The polymer that we use for pyrolysis is allyl-hydridopolycarbosilane (AHPCS), which converts to SiC with a nearly stoichiometric ratio of Si:C. Microporous SiC membranes are prepared by the pyrolysis of thin AHPCS films coated, using a combination of slip-casting and dip-coating techniques, on tubular SiC macroporous supports.

We have also developed a novel reactor system, termed the hybrid adsorbent-membrane reactor (HAMR), which couples the reaction and membrane separation steps with adsorption on the reactor and/or membrane permeate sides. We study the HAMR system for *on-site* or *on-board* hydrogen production in place of the more conventional technologies used for such applications. We have used microporous and metal-membranes and CO_2 hydrotalcite-type adsorbents, and we have studied both the water-gas shift and steam reforming reactions.

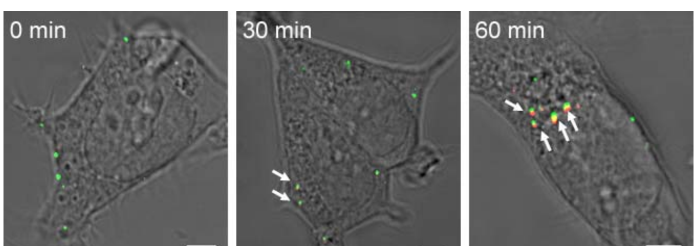
Return to Faculty Research Areas

Pin Wang

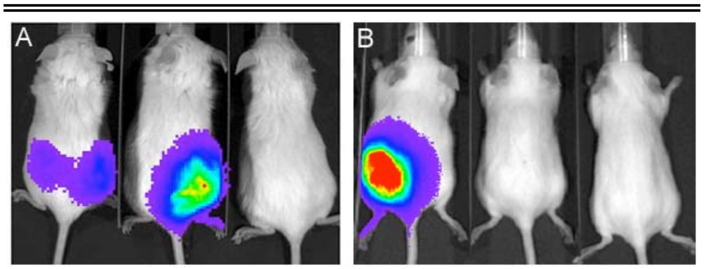
Engineering Immunity, Biomolecular Engineering, Gene Therapy



Our research focus is to apply engineering design principles to the field of nanomedicine and gene medicine, allowing us to develop novel methods for combating diseases such as HIV and cancer. One example is to develop novel gene delivery technology for the targeted modification of immune cells.



Many advanced experimental tools such as confocal microscopy are used to investigate molecular events at the nano scale in cells. We are able to monitor the trafficking of nano-sized particles in live cells. As engineered particles travel across the cells, they can fuse with endosomes to empty the genetic materials into the cytosol. Yellow particles denoted by arrows indicate that the particles have fused to endosomes.



Non-invasive live animal imaging can be employed to monitor the *in vivo* delivery of nano-particles. The image on the left (A) shows that the engineered nano-particles can specifically target tumor cells. The image on the right (B) shows that the engineered nano-particles can serve as vaccine carriers and that vaccination can eradicate pre-established tumors.

Our research interest is to develop new approaches for engineering gene delivery vehicles for targeted and *in vivo* gene therapy. We are able to manipulate the surface of certain viral particles, one form of nanoparticles, to achieve the delivery of therapeutic genes to targeted cells. This approach has successfully been taken to target dendritic cells (DCs), T cells, B cells, and stem cells. These cells are involved in the body's immune system and by targeting them we can equip them with vital defenses against virulent diseases and different types of cancers. This specific and carefully optimized approach has the potential to treat previously incurable diseases.

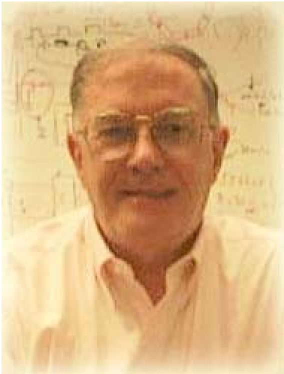
One example of a project currently pursued is DC targeting. The aim of the work is to create novel DC-based vaccines. The lab has created nano-particles that are able to target DCs *in vivo* to deliver antigens for cancer cells and infectious viruses. Once these antigens are delivered into the DCs, they are presented to T cells, which identify and destroy harmful intruders to the body. Through their interactions with the DCs, T cells are taught to recognize the antigens on the DC surface as dangerous ones. By employing the body's innately efficient mechanisms, we can now "teach" the immune system to be aware of and attack cancers, as well as other diseases, including HIV.

Another approach being taken in the lab involves hematopoietic stem cells (HSCs). These cells develop into blood cells, including T cells and B cells. Through gene therapy to HSCs, the immune system can be conditioned to treat and resist HIV, cancer, metabolic disorders, and inborn errors of metabolism. Our engineering approach has been successful in producing viral particles to target CD34+ (the distinguishing marker for HSCs) cell lines both *in vitro* and *in vivo*.

Return to Faculty Research Areas

Peter Will

MEMS

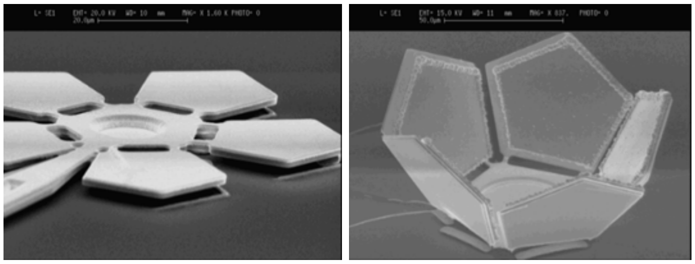


Peter Will's current research is on MEMS-based voxels for nano-encapsulation of material and on various aspects of Microsatellite Systems particularly on time and fuel optimal attitude control systems and in the development of vector field methods for distributed control of formations of spacecraft.

Voxels

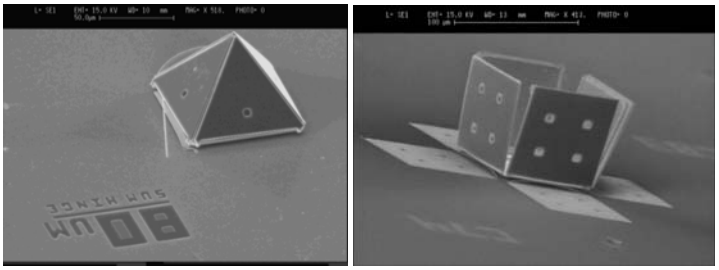
MEMS–based volume encapsulation or voxel devices were fabricated in the MUMPS process. The release, permalloy plating and subsequent magnetic erection from the plane were done at USC. Devices at a variety of sizes were built ranging from 20 to 80 microns on a side. The long term goal is the encapsulation of small volumes of materials such as therapeutic drugs.

Open structures



Voxels: left flat as printed b erected as a lotus blossom-shaped bowl

Closed Structures



Pyramid and Open box

Return to Faculty Research Areas

Jongseung Yoon

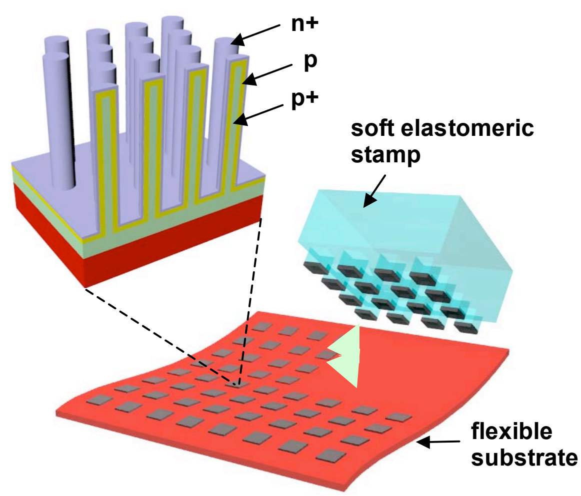
Micro/Nanostructured Materials; Energy Harvesting, Electronic, Optoelectronic, and Photonic Materials and Devices; Nanotechnology; Nanofabrication

Our group will seek fundamental understanding of properties of micro- and nanostructured materials and exploit them as functional building blocks for applications in energy harvesting, electronics, optoelectronics, photonics, and sensor technologies. We are interested in developing materials and fabrication strategies that can create hybrid and multi-functional devices in unusual platforms and characteristics, enabled by various top-down and bottom-up micro/nanofabrication techniques, deterministic printed assembly, together with heterogeneous integration of dissimilar materials. Our research efforts are highly interdisciplinary, spanning various science and engineering disciplines from materials science, physics, and chemistry to electrical engineering.

Nanostructured semiconductor materials represent alternative to traditional bulk and thin film devices in photovoltaics. Of particular interest are micro-/nanowire solar cells due to their potential advantages including extremely efficient carrier collection, effective light trapping, and reduced demand for materials purity. One of our research areas is the integration of micro- and nanowire photovoltaic devices using wafer-based single crystalline inorganic materials. We use soft nanoimprint lithography and block copolymer self-assembly to generate highly ordered nanoscale patterns. Subsequently, we transfer such nanopatterns to photoactive materials and implement device functionalities using conventional microfabrication techniques. The resulting micro- and nanowire solar cells are integrated on diverse classes of foreign substrates to form modules that can provide desirable characteristics including ultrathin, lightweight, large area, and flexible construction, together with simultaneously optimized carrier collection and photon absorption, and cost-effectiveness.

Fundamental limit of solar energy conversion efficiency in single junction photovoltaic devices arises from the use of materials that can only absorb a fraction of solar spectrum corresponding to the semiconductor energy gap. One of the most successful approaches to circumvent such efficiency limit has been to use multiple number of series-connected semiconductor materials with different bandgaps, which can utilize different portions of solar spectrum and therefore achieve higher efficiency. Another area of our research is the development of alternative integration pathway for multijunction solar cells through additive, deterministic transfer printing techniques. This approach with materials of optimally combined bandgap energies has potential to minimize restrictions associated with epitaxially grown monolithic systems in terms of quality and types of materials that can be employed, but also to achieve improved performance, reduced cost, as well as unconventional integration platforms.

Other research interests in the group include nanophotonics-enabled optoelectronic devices, and printed arrays of micro/nanostructured thermoelectric materials for applications in waste heat recovery and cooling for microelectronics.



Schematic illustration of printed arrays of micro/nanowire photovoltaic cells in ultrathin, large area, and flexible configuration.

Return to Faculty Research Areas

Yannis C. Yortsos

Chemical and Petroleum Engineering

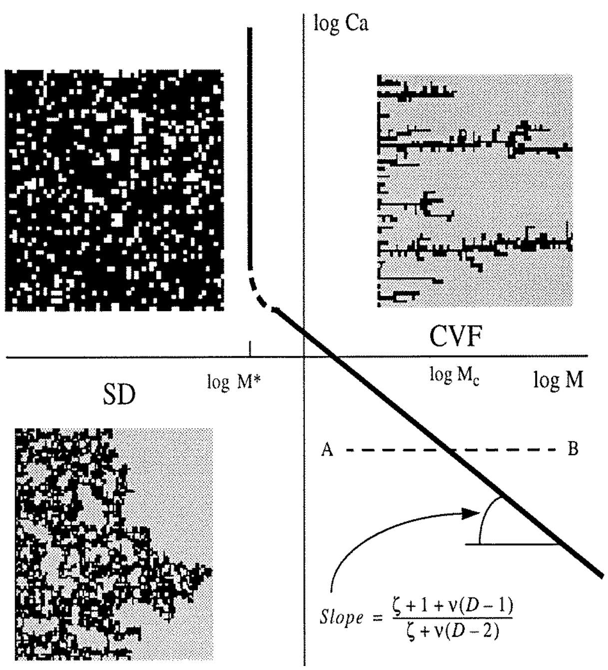
Yannis C. Yortsos is the Dean of Engineering at the USC Viterbi School of Engineering and holds the Zohrab Kaprielian Deans' chair. He is also the Chester F. Dolley Professor of Petroleum Engineering and Professor of Chemical Engineering in the Mork Family Department of Chemical Engineering and Materials Science.

He has done research in fields that include fluid flow, transport, and reaction in porous media, viscous flows in porous media geometries, phase change in porous media, with applications to the recovery of subsurface fluids (oil recovery, soil remediation).

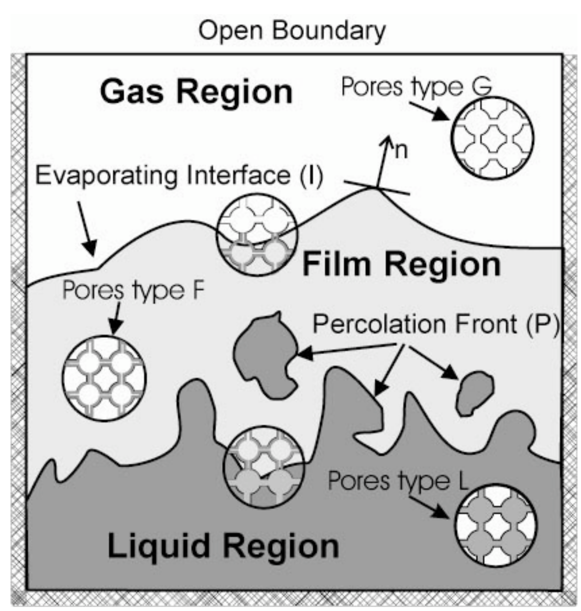
Yortsos has extended the application of percolation theory to study the fundamental dynamics of a wide range of transport processes in porous materials. Examples of his studies include delineating immiscible flow regimes in porous media (below left) and evaporation of volatile liquids residing in porous media (below right).

Additional specific examples of research activities in relation to flow and transport in porous media include:

- Miscible flows in Hele-Shaw cells
- Vapor-Liquid Flow in Porous Media
- Transport and Displacement in Heterogeneous and Fractured Media
- Scale-Up of Displacement Processes in Heterogeneous Media
- Flow of Fluids with Yield Stress in Porous Media
- Darcian Dynamics
- Heterogeneity Identification
- Filtration Combustion



Delineation of immiscible flow regimes in porous media (Phys. Rev. Lett. 79, 4581-4584 (1997)).



Evaporation and diffusion of volatile liquids in porous materials (AIChEJ 50 (11), 2721-2737 (2004).

Return to Faculty Research Areas