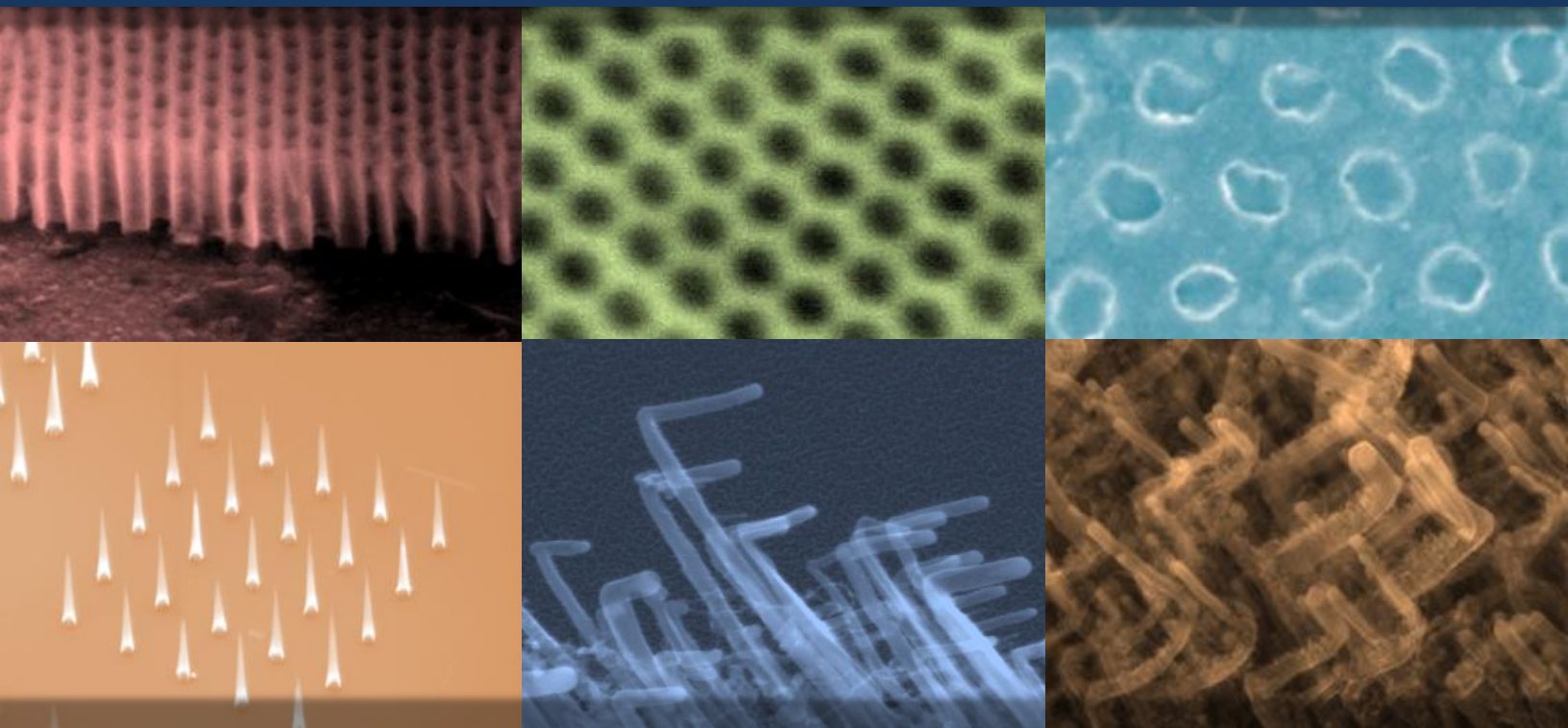


Fall 2012

MATERIALS NEWS

UCSD Materials Science & Engineering Newsletter



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Layout and Design: Youngjin Kim
Printing: Replica La Jolla

LETTER FROM THE DIRECTOR

This is the YR 2012 newsletter describing UC San Diego's Materials Science & Engineering (MSE) Program, and I hope you enjoy reading about education and research activities in our program.

The MSE Program at UC San Diego is a university-wide, highly interdisciplinary program with more than 85 participating UCSD faculty members. The professors and students in our program come from various divisions of UCSD, including the Jacobs School of Engineering (Departments of Electrical and Computer Engineering, Mechanical and Aerospace Engineering, Structural Engineering, Bioengineering, Nanoengineering), Division of Physical Sciences (Department of Physics, Department of Chemistry & Biochemistry), Division of Biological Sciences, the School of Medicine, and the School of Pharmacy.

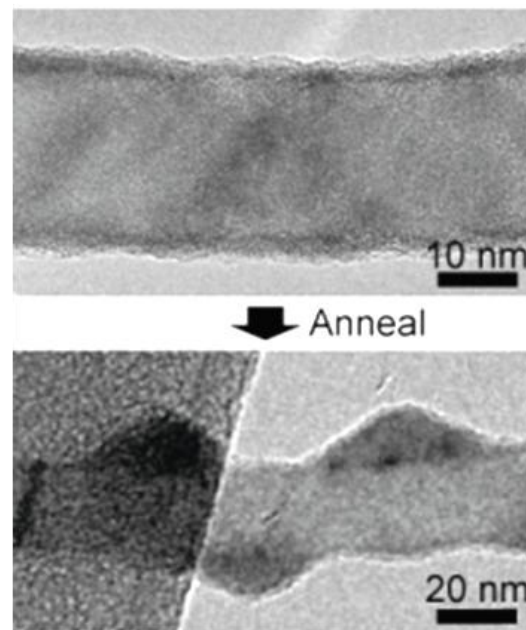
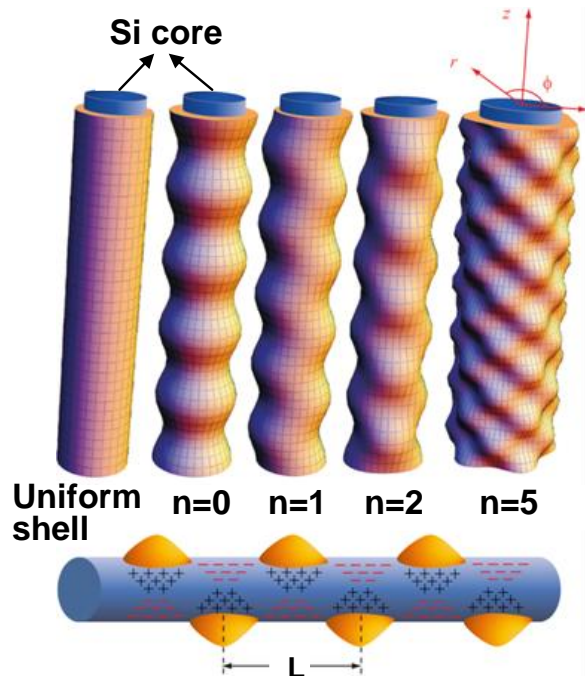
Our MSE faculty members are mostly outstanding in their research and education career, with the faculty now including 8 National Academy of Engineering, 5 National Academy of Sciences, 3 Institute of Medicine members, and the prestigious National Medal of Science Awards in recent years to Prof. Shu Chien and Prof. Marye Anne Fox who are also our MSE members. Having such an excellent quality of faculty, combined with one of the highest per faculty research grants in the nation, provides a stimulating environment for our graduate students working toward their MS and PhD degrees. The total number of our graduate students in Materials Science and Engineering is now over ~130. UCSD's Materials Science & Engineering (MSE) is ranked 14th among all Materials Science doctoral programs in the United States by the prestigious National Research Council (NRC) data-based assessment. I am always proud of our faculty and graduate students in the MSE program for their enthusiasm toward high quality education and research. With future newsletters, we will continue to share the latest information on academic, research, and career progress of our faculty, students, postdocs, and alumni from our MSE Program.



A handwritten signature in black ink that reads "Sungho Jin". The signature is fluid and cursive.

Sungho Jin

Director, UCSD Materials Science & Engineering Program
Distinguished Professor of Materials Science



(Left) Schematic of possible surface instability modes of Ge shell on Si core nanowires, and (Right) TEM microstructural confirmation of such an anti-correlated Ge dot array.

Feeling stressed? Get Organized!

When you pound a drum, its surface strain propagates and resonates through the membrane in a regular tonal pattern giving the distinctive and beautiful drum sound. By using such correlated and propagated strain in nanomaterials, Professor Jie Xiang in the ECE department and MSE student Soonshin Kwon have recently reported for the first time self-organization of periodic nanocrystals on the surface of a cylindrical nanowire. They used a single crystal Si nanowire as substrate and tried to grow Ge, another semiconductor, epitaxially on the Si surface. A Ge island formed on one side creates tensile strain within the Si immediately under it due to the larger lattice mismatch of Ge compare to Si (+ signs). This in turn leads to compressive strain in Si at the bottom side (- signs), much in the same way as the convex and concave surfaces of a bent pipe. As a consequence further Ge deposition at the bottom side will occur which tends to avoid the compressively strained (-) surfaces while preferentially growth occurs at the tensile strained

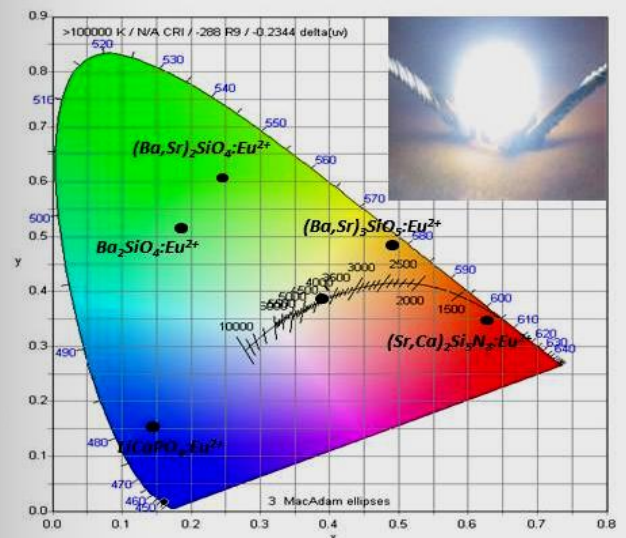
(+) region, resulting in an anti-correlated zig-zag organization of Ge dots on Si surface in order to reduce the total elastic energy of the system. They found several different modes of Ge island ordering on the Si nanowire backbone depending on the core diameter. Moreover, simply heating up a uniform Ge shell layer converts it to discrete Ge island arrays. The impact of this finding is twofold: not only does it prove that strain engineering in nanomaterials can provide a unique driving force towards self-organization of periodic nanostructures, but perhaps more profoundly, the periodic stress underlying each QD and the resulting modulation of electro-optical properties inside the nanowire backbone promise to provide a new nanostressor-superlattice platform for novel mechano-electronic, thermoelectronic, and optoelectronic devices.

The researchers involved in this project include Prof. Jie Xiang of ECE Department, Soonshin Kwon, Zack Chen and Jihun Kim. Soonshin Kwon is a PhD student in the MSE program. (see the published article, "Misfit-Guided Self-Organization of Anti-correlated Ge Quantum Dot Arrays on Si Nanowires", S. Kwon, Z.C.Y.Chen, J. Kim and J. Xiang, Nano Letters, 12, 4757-4762, 2012.)

UC San Diego Team Succeeds in New Phosphor Synthesis for Near UV-Emitting LEDs

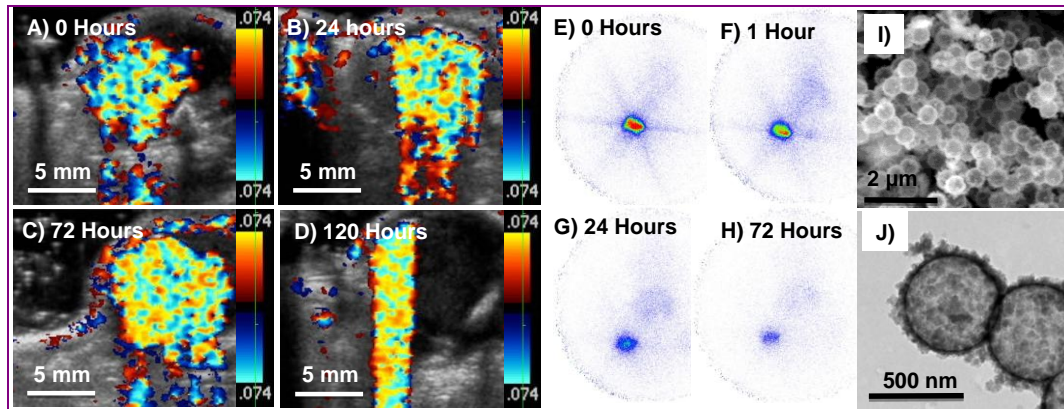
The results of our US Department of Energy project No. EE0002003 was selected by our DOE Program Manager for inclusion in the DOE report summarizing Solid State Lighting Program for Fiscal Year 2012.

Graduate students Jinkyu Han and Jae Ik Choi under the guidance of Professors Joanna McKittrick and Jan Talbot are working toward developing blue, red and green-emitting phosphors with high quantum efficiency (QE) exceeding 95 percent in response to excitation in the spectral region of 380-400 nm. Most LEDs used for general illumination today are blue LEDs, converted to white light using phosphors. UCSD's novel approach is to develop phosphors for a near ultra violet (UV) LED instead of a blue LED, because near UV LEDs have fewer binning and current droop issues. Also, the near UV LEDs would rely completely on the phosphors for the generation of the white light, which would give better control of light quality and color temperature. The UC San Diego team, together with their partner OSRAM Sylvania, has made excellent progress, with the QE reaching 88 percent for blue phosphor, 90 percent for green/yellow, 90 percent for orange, and 90 percent for red.



Schematic solid state lighting, actual device parts, and a plot of phosphor performance for various new phosphor compound materials.

Perfluoropentane Gas and Liquid Filled Hollow Silica Micro/Nano Spheres for Ultrasound Guided Surgery and HIFU Therapy



Longevity and Biodistribution of Locally injected Perfluoropentane vapor filled 500 nm hollow Fe-SiO₂ Nanoshells in Py8119 Breast tumor bearing Nu/Nu Mice. 500 nm Fe-SiO₂ nanoshells were injected directly into the tumor and imaged by color Doppler ultrasound. A) Imaging immediately after injection. B) Image 24 hours post injection. C) Imaging 72 hours post injection. D) Imaging 120 hours post injection. Nanoshells were also radiolabeled with In-111-DTPA and imaged by γ -scintigraphy after intratumoral injection. E) Imaging immediately after injection. F) Image 1 hours post injection. G) Imaging 24 hours post injection. H) Imaging 72 hours post injection. I) Scanning Electron Microscopy of nanoshells. J) TEM of nanoshells.

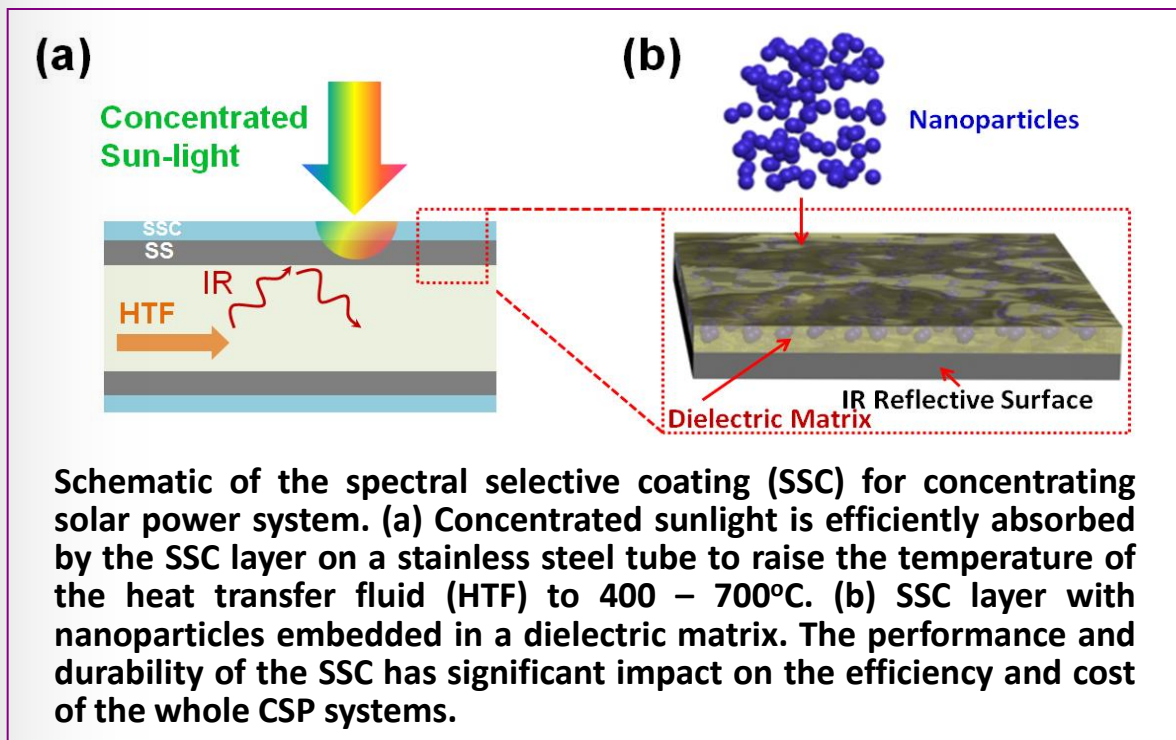
The reported positive margin rate from wire localized excisions of breast cancers is approximately 20-50%; however, by pre-operatively injecting a radio active seed into the tumor under CT guidance, the excision rate is halved because the surgeon can constantly reorient the dissection to place the seed in the center of the specimen. Unfortunately, radioactive seed localization has several safety challenges, only single foci can be localized, and incisions are required to implant the seeds, so it is rarely employed. As a safe alternative, gas-filled hollow Fe-doped silica particles have been developed, which can be used for ultrasound-guided surgery even for multiple foci. The function of the Fe doping is to render the silica shells biodegradable. The particles are synthesized through a sol-gel method on a polystyrene template, and subsequently calcined to create hollow, rigid microspheres.

The Fe-doped silica shell is derived from tetramethoxy orthosilicate (TMOS) and iron (III) ethoxide, which forms a rigid, mesoporous shell upon calcination. The microspheres are filled with perfluoropentane (PFP) vapor or liquid. The fluorine phase is contained within the porous shell due to its extremely low solubility in water. Considerable testing of particle functionality, signal persistence and acoustical properties have been performed in various phantoms including ultrasound gel, chicken breast, and excised human mastectomy tissue. *In vitro* studies of these have

shown that continuous particle imaging time is up to approximately 45 minutes, and will persist for over five days. Furthermore, preliminary *in vivo* particle injection longevity studies have been performed in a rabbit model which are consistent with *in vitro* data showing signal presence even five days post injection. These silica spheres may be used as a sensitizing agent in high intensity focused ultrasound (HIFU). Traditional ultrasound agents pose several potential drawbacks such as poor *in vivo* persistence (minutes) and high risk (cardiac complications) during continuous perfusion. Preliminary *in vitro* results in HIFU ablation in an agar tissue phantom model suggest that very few particles are needed in order to develop a sensitizing effect to HIFU (approx. 1-10 $\mu\text{m}/\text{ml}$ particles/agar varying by particle size). A novel technique has been developed to fill the particles with perfluorocarbon liquid which vaporizes upon exposure to HIFU thereby increasing the sensitivity compared to gas filled particles.

Contributors to this research article include Alexander Liberman¹, H. Paul Martinez², Zhe Wu³, Christopher Barback³, Sarah L. Blair⁴, Yuko Kono³, Robert F. Mattrey³, William C Trogler², Andrew C. Kummel¹ (1. Materials Science and Engineering Program, 2. Department of Chemistry and Biochemistry, 3. Department of Radiology, and 4. Moores Cancer Center, UC San Diego).

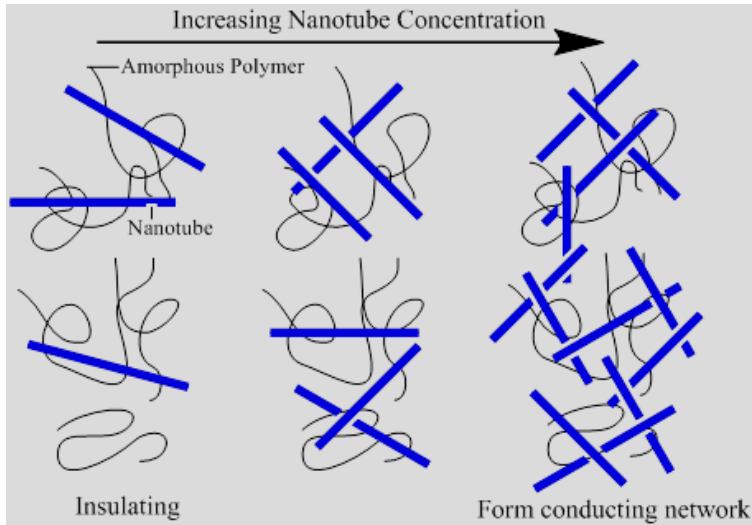
Nanostructured Coating for Solar Energy



A team of materials researchers at UCSD is developing a new low-cost and scalable process for fabricating spectrally selective coatings (SSCs) to be used in solar absorbers for high-temperature concentrating solar power (CSP) systems. The project is part of the US Department of Energy Sunshot CSP Research and Development program, aiming to achieve the grid-parity for solar energy by 2020. The SSC layer is a critical component that maximizes solar thermal energy absorption to enable high-temperature and higher-efficiency operation of CSP systems. The research team is working to demonstrate a bandgap adjusted semiconductor nanoparticle-based coating that can achieve high solar absorptance and low infrared emittance, leading to high thermal conversion efficiencies and increased temperature ranges for heat-transfer fluids. This research employs the novel use of surface-protected semiconductor nanoparticles, which are fabricated by a highly scalable particle synthesis method with desired size distributions. By engineering the material properties and morphologies of the nanoparticle coating, the fabricated SSCs simultaneously possess the metrics of high performance, low cost, and high-temperature durability.

The research team undertaking this effort includes Materials Science graduate students Jaeyun Moon, Taekyung Kim, Bryan VanSaders, Danyong Lu, and Professors Renkun Chen, Sungho Jin, and Zhaowei Liu.

Applying Information Theory Principles to Networks of Nanostructures, with Implications to Enhancing the Electrical and Thermal Conductivities of Polymers

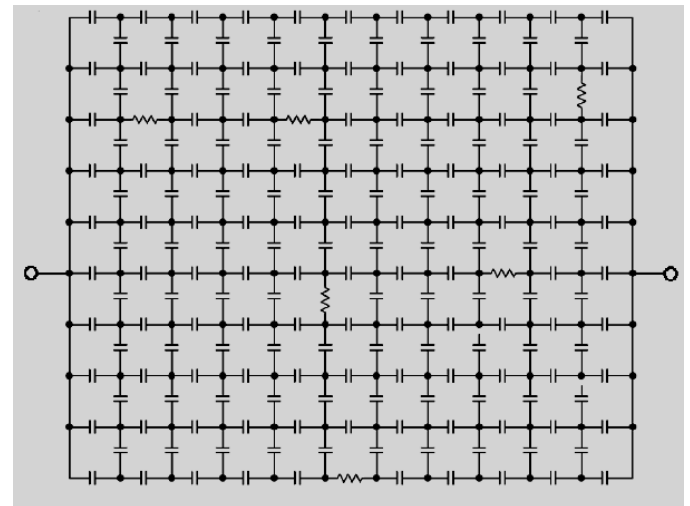


The figure illustrates that increasing the concentration of carbon nanotubes leads to the formation of an electrically and thermally connected network, with the conductivity following a power law relation.

Networks and connections are ubiquitous in our daily lives and span the range from the interpretation of the internet as a large interconnected web to the arrangement of nanostructures in a macroscopic material. Steve Pfeifer, a graduate student, working with Professor Bandaru, has extended the paradigm of finding networks to that of looking at the inter-connectedness of nanotubes in polymers. The mathematical problem of analyzing the minimal concentration of carbon nanotubes (CNTs) necessary to form a percolating electrical and thermal network was solved and experimentally verified. CNTs were chosen for their unique one-dimensional elongated structure, which enables easier connections to be made with smaller volume content. For example, it was found that just 0.01% of nanotubes (with a diameter of 1 nanometer and a length of 1 micron) was adequate to form a network with the consequence that when such nanostructures are dispersed in a polymer matrix, the electrical conductivity can be enhanced by *ten orders of magnitude* over that of the host. Information theory based principles such as minimizing the relative entropy of the nanostructure-polymer distribution.

The Akaike information criterion were then applied for obtaining an appropriate and optimized electrical circuit model of the nanotube-polymer composite, whereby a penalty was imposed for increasing the number of fitting parameters.

The work, sponsored by the National Science Foundation, has immediate applications to spray-on conductive polymer composites for electromagnetic interference shielding, and long term implications to network and graph theory and statistical physics, determining percolation thresholds in sociological interaction thresholds (e.g., how many contacts are necessary to spread information from one point to another), etc. Pfeifer and Bandaru have applied for a patent on the developed mathematical algorithms and the work has been published in *IEEE Transactions in Nanotechnology* and *Electrochemical and Solid State Letters*.



Information theory based principles combined with frequency dependent electrical impedance models enabled the creation of an optimized electrical model for a given polymer-nanotube composite. The figure above depicts 97 capacitors and 3 resistors as representative of the dielectric/polymer space (capacitors) between the conducting nanotubes (resistors)

Lunar Cement and Lunar Buildings?

Professor Yu Qiao at UCSD is working with NASA to develop a novel structural material – lunar cement, by using lunar soils. The technology, once developed, will enable building large-scale bases, outposts, power plants, and other research/exploration facilities and equipment on the Moon. It may also be extended to other planets and planetary satellites. The key concept is to use a minimum amount of binder, which may be prepared on and transported from the Earth, to combine lunar soil grains, which may be treated through simple and energy efficiency procedures, into load-carrying structural components.

The personnel involved in this project include Prof. Qiao, Dr. Gang Wang, Dr. Weiyi Lu, and Mr. Derek Chen. Derek Chen is a Ph.D. student from the Materials Science & Engineering Program at UCSD.

Lunar Cement?

— Building Buildings Using Lunar Regolith



Professor Yu Qiao

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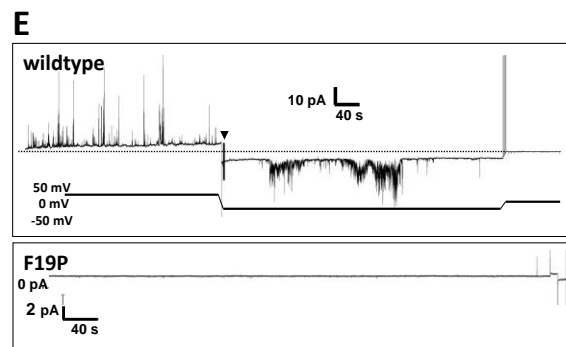
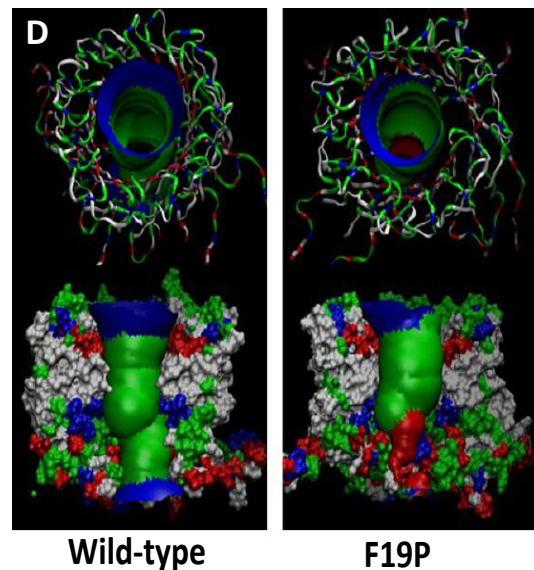
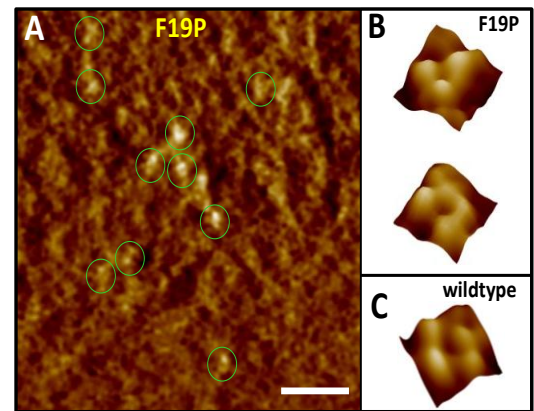
Phone: 858-534-3388 ♦ Email: yqiao@ucsd.edu

Unraveling Therapeutic Targets in Alzheimer's Disease

This article deals with a study of toxic amyloid channels by atomic force microscopy, electrophysiology, and MD simulations. Alzheimer's disease (AD) is a misfolded protein disease characterized by the accumulation of β -amyloid ($A\beta$) peptide as senile plaques, progressive neurodegeneration, and memory loss. AD pathology is linked to the destabilization of cellular ionic homeostasis mediated by toxic pores made of $A\beta$ peptides. Understanding the exact nature by which these pores conduct electrical and molecular signals could aid in identifying potential therapeutic targets for the prevention and treatment of AD. Materials Science and Engineering graduate student Laura Connelly and Prof. Ratnesh Lal of bioengineering together with collaborators Hyunbum Jang and Ruth Nussinov at the NIH have studied the structure-activity relationship of these toxic pores through materials characterization, biophysical techniques, and computer modeling. Laura and her fellow researchers examined the electrical activity of $A\beta_{1-42}$ pores by conductance measurements in planar lipid bilayer (PLB) and 3D structure by atomic force microscope (AFM). The imaged structures are compared with molecular dynamic simulation (MDS) models to predict its conformation as a function of amino acid sequence.

Site-specific amino acid (AA) substitutions in the wildtype $A\beta_{1-42}$ peptide yield information regarding the location and significance of individual AA residues to its characteristic structure-activity relationship. MD simulations predicted this substitution, abbreviated F19P, to form a pore with a compromised structure, collapsed at the inner lining, which would inhibit its activity. This prediction was supported by pore-like structures of F19P observed in a lipid bilayers by AFM. It is suggested that the F19 residue may be a viable target for drug development studies aiming to inhibit amyloid- β from inducing ionic destabilization toxicity. (see Laura Connelly, Hyunbum Jang, Fernando Teran Arce, Srinivasan Ramachandran, Bruce L. Kagan, Ruth Nussinov, Ratnesh Lal, *J. Biochemistry* 51, 3031 (2012).)

(Panel A) Amplitude AFM images of F19P $A\beta_{1-42}$ incorporated into DOPC bilayers on mica. (Panel B) Individual pores from the amplitude images were selected and resolved into multimeric structures. The pores appear characteristic of (Panel C) wild-type $A\beta_{1-42}$, as a surface structure image, do not exhibit any indication of a compromised pore structure. (Panel D) Averaged pore structures calculated with HOLE38 embedded in the average barrel conformations during the simulations $A\beta_{1-42}$ barrels. In the angle views of the pore structure (top cartoons in each panel), whole barrel structures are shown with the ribbon representation. In the lateral views of the pore structure (bottom cartoons in each panel), cross-sectioned barrels are given in the surface representation. In the peptide, hydrophobic residues are colored white, polar and Gly residues green, positively charged residues blue, and negatively charged residues red. For the pore structures in the surface representation, red denotes pore diameter of $d < 1.4$ nm, green denotes pore diameter in the range, $1.4 \text{ nm} \leq d \leq 2.0$ nm, and blue denotes pore diameter of $d > 2.0$ nm. (Panel E) Electrical recordings from PLB show characteristic activity of the wild-type $A\beta_{1-42}$ compared to no activity for the F19P mutation.



Student Awards & Honors

Laura Andersen received the 2012 ASM Abe Hurlich Award from the San Diego chapter of ASM International (American Society of Materials). The award was established in memory of Abe Hurlich, a member and past-chair (1960) of the chapter, and past-president of ASM International (1977). The award recognizes one local student who exhibits outstanding merit in scholarship, leadership, and service, and consists of a \$1200 scholarship, one-year ASM membership, and a medallion. Laura is a second year student in the Materials Science and Engineering Ph.D. program in Prof. Ken Vecchio's group, researching metallic glasses. Laura's extensive research experience, academic excellence and community involvement were highlighted at the 2012 ceremony, in which she was presented with the award.

MSE Faculty Award

National Academy of Engineering

Professor Michael Baskes Elected to NAE

Professor Baskes, an Adjunct Professor in the Mechanical & Aerospace Engineering Department and a participating faculty member in the Materials Science & Engineering Program was elected to NAE "for contributions to the embedded atom method for predicting the structure and properties of metals and alloys." He uses computational methods to investigate, model and predict material properties.



MSE New Faculty



Patrick Mercier (Dept of Electrical and Computer Engineering)

Research in the Mercier's group explores Energy-efficient Microsystems, circuit and system design, biomedical applications and energy harvesting architectures.



Jian Luo (Department of NanoEngineering)

Professor Luo's group has focused on the Interfacial thermodynamics, Surfaces, grain boundaries, and hetero-phase interfaces, Nanoscale interfacial (surficial or intergranular) films, Materials characterization (TEM, HRTEM., XRD etc.), Nanostructured thin films: spin and dip coating; nanoclay-based multilayers, Optical materials and fibers, Continuum-level material and optical simulations.



Shengqiang Cai (Dept of Mechanical & Aerospace Engineering)

Professor Cai's research focuses on the field of Mechanics of artificial and biological soft materials, Energy harvesting and storage, Micro-fabrication techniques of polymeric structures and soft/stiff hybrid structures, Deformable acoustic and electromagnetic metamaterials.

New Graduate Students 2012

Welcome 40 New Graduate Students who joined our Materials Science & Engineering Program this academic year.

Ahn, Chi Hyung
(Seoul National Univ)

Chuang, Chen
(National ChengKung Univ)

Chuang, Ying Sheng
(National ChengKung Univ)

Chun, Dongwon
(Yonsei Univ)

Cyrus Rustomji
(UC San Diego)

Hahn, Eric Nicholas
(Cal Poly, SLB)

Huang, Keyuan
(Sun Yat-sen Univ)

James Cahill
(Alfred Univ)

Jeon, Inho
(Hanyang Univ)

Jiajia Huang
(Clemson Univ)

Kim, Jayoung
(Yonsei Univ)

Kim, Young Hun
(Yonsei Univ)

Kim, Young Jin
(UC San Diego)

La, Rui
(Univ Florida)

Lee, Chihying
(Nat'l Tsing Hua Univ)

Li, Ziyang
(Univ Florida)

Lin, Hunghsi
(TsingHua Univ)

Liu, Chang
(Fudan University, Shanghai)

Mojtaba Samiee
(Clemson Univ)

Naixie Zhou
(Clemson Univ)

Naso, Angela
(Univ Virginia)

Olson, Scott
(Lehigh Univ)

Park, Sang Wook
(Stanford Univ)

Ren, Tianqi
(Michigan State Univ)

Sardashti, Kasra
(Alexander Univ, Erlangen)

Seo, Kyungah
(GIST)

Sheng, Wangzhong
(Cornell Univ)

Sherman, Vincent Robert
(UC San Diego)

Shi, Dinghao
(Shanghai University)

Shi, Yang
(Dalian Univ)

Song, Jing-Jin
(Tsing Hua Univ)

Vansaders, Bryan James
(Rutgers Univ)

Wang, Bin
(Zhengzhou Univ)

Wang, Kangwei
(Natl Taiwan Univ)

Yuanyao Zhang
(Clemson Univ)

Zhang, Cheng
(Beijing Univ. Sci & Tech)

Zhang, Minghao
(Chinese Acad. of Sci)

Zhang, Qing
(Jilin Univ)

Zhang, Tiantian
(Arizona St Univ)

Zhu, Haoqing
(East China Univ. Sci & Tech)

About the MSE Department Graduate Coordinator

Charlotte Lauve was born in Germany and raised in Texas and California in US. She grew up in San Diego, and has done extensive traveling, camping, fishing, surfing and horse back riding. Charlotte has worked at UCSD for almost 23 years as the Graduate Coordinator for the MSE Graduate Program.

About The Editor:

Duyoung Choi is a fourth-year graduate student in the Material Science & Engineering at UCSD. In 2003, he earned a Bachelor's of Science in Chemical & Biological Engineering, and Master's Degree in Chemical Engineering at the Inha University, South Korea. He is currently conducting research in Prof. Sungho Jin's group on preparation, properties and applications of periodic nano arrays of metallic, ceramic and polymer materials.

We would love to hear the achievements and milestones from the UC San Diego Materials family that comprises students, alumni, faculty, visiting scientists and staff for inclusion in our next newsletter.

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Graduate Program Representative

UC San Diego Materials Science & Engineering Program

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