

MATERIALS RESEARCH INSTITUTE BULLETIN

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Computation from A to Z **

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Message from the Director



In this issue of *Focus on Materials*, we will touch on a few of the many facets of computer technology and computational science as they relate to materials discovery and application. The history of computing is a remarkable story that is still unfolding. In fact, even after 60 years of rapid progress, we may still be reading only the first chapter. Meanwhile, researchers in the Materials Research Institute and Penn State are in the forefront of transistor development for next generation computers, as well as using computational techniques to develop advanced materials and materialsbased technologies.

It has been often noted that a new material takes 15-20 years

to reach market. The typical trial-and-error approach to finding new materials suitable for a specific application is slow and expensive. Consequently, it has become prohibitive to develop a truly new material, while advancing an existing material is the more common industrial approach to new materials. This is where computational techniques can offer tremendous benefits. In this issue, we focus on a pair of faculty researchers who use simulations at different size scales to help experimentalists plan their experiments and interpret their data. We also provide a glimpse at what it takes to create a new type of transistor, one that in a few years may be in many of your desktop and mobile devices.

An exciting new project that will attempt to develop an artificial visual cortex on silicon, also known as a smart or cognitive camera, that could help drivers avoid accidents, visually impaired people navigate their surroundings, or let police recognize criminal activities was recently funded by the National Science Foundation Exploration Program with a \$10 million award over five years. Penn State is the lead on this project, which includes some of the top university researchers from across the country.

And for those who couldn't make it to this year's very successful Materials Day event, we offer a photo montage and brief summary of what you missed. There is more online, so visit us at **mri.psu.edu**.

Sincerely,

Carlo Pantano

Director of the Materials Research Institute and Distinguished Professor of Materials Science and Engineering

To access the materials expertise at Penn State, please visit our Materials Research Institute website at **www.mri.psu.edu** or the Office of Technology Management website at **http://www.research.psu.edu/offices/otm**



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Snapshots are brief summaries of significant materials-related breakthroughs by MRI researchers. More information is available by visiting the links at the end of each summary.

FOCUSING LIGHT BEAMS WITH TINY BUBBLES



A nanoscale light beam modulated by short electromagnetic waves, known as surface plasmon polaritons – labelled as SPP beam – enters the bubble lens, officially known as a reconfigurable plasmofluidic lens. The bubble controls the light waves, while the grating provides further focus. Credit: Tony Jun Huang, Penn State

Researchers at Penn State, with help from colleagues at Northeastern and MIT, have made lenses out of water bubbles that can focus beams of light on an electronic chip, paving the way for improvements in on-chip biomedical devices and super resolution imaging.

The benefit of the water droplet approach over solid state devices is the ease of reconfiguring the lens. The researchers can reconfigure the bubble's location, size, and shape by adjusting the power of a laser shone on the bubble.

"In addition to its unprecedented reconfigurability and tunability, our bubble lens has at least one more advantage over its solid-state counterparts: its natural smoothness," said Tony Huang, professor of engineering science and mechanics at Penn State. "The smoother the lens is, the better the quality of the light that passes through it."

In addition to Huang, the Penn State team included lead author Chenglong Zhao, postdoctoral fellow in engineering science and mechanics, and graduate student Yanhui Zhao, engineering science and mechanics. The paper appeared in the journal Nature Communications.

For more information, read the news release by Hannah Cheng on the MRI News Page: http://www.mri.psu.edu/news/.

SYNTHETIC POLYMERS **ENABLE CHEAP, EFFICIENT, DURABLE ALKALINE FUEL CELLS**



A membrane electrode assembly being inserted into a fuel cell testing stand. By creating several variations of membranes and studying them under similar conditions, the research team can predict the most optimal structure in an active and stable fuel cell. Credit: Patrick Mansell, Penn State

CHEMICAL ENGINEERS' RESEARCH MAY LEAD TO INEXPENSIVE, FLEXIBLE SOLAR CELLS

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A new polymer anion exchange membrane developed in the lab of Michael Hickner, associate professor of materials science and engineering at Penn State, could make fuel cells more affordable in the future. Current proton exchange membrane fuel cells (PEMFC) require expensive catalysts, such as platinum, combined with perfluorinated membranes and corrosion-resistant cell hardware, all of which drive up the cost. Hickner's membrane was developed to be used in an alkaline fuel cell, which can operate with non-noble metals or inexpensive metal oxides as catalysts, greatly reducing the cost of the devices.

Hickner worked with Chao-Yang Wang, distinguished professor of mechanical engineering and professor of materials science and engineering, to test the membrane. Also reporting on their findings in the Journal of the American Chemical Society were Nanwen Li, postdoctoral researcher in material science and engineering, and Yongjun Leng, a research associate in mechanical and nuclear engineering.

The Advanced Research Projects Agency-Energy at the U.S. Department of Energy, funded this project in collaboration with Proton OnSite, a leading membrane electrolyzer company based in Connecticut. For more information, read the news release by Hannah Cheng on the MRI News Page: http://www.mri.psu.edu/news/ or read the paper at http://pubs.acs.org/doi/pdf/10.1021/ja403671u.

Organic solar cells are potentially less expensive and certainly more flexible than the inorganic solar cells made of crystalline silicon. Although there are several organic solar cells on the market in niche applications, the majority employ fullerene acceptors that are difficult to scale up. Enrique Gomez, a chemical engineer at Penn State, and a team from Rice University, Argonne National Laboratory, and Lawrence Berkeley National Laboratory have controlled the microstructure and interface of the polymer solar cells so that the molecules link together in better ways. The hope is to make flexible organic solar cells that can be printed as easily as newspapers. Currently at only three percent efficiency,

the researchers believe they can do better. However, their prototype shows that flexible organic solar cells are feasible. Their results appeared in the American Chemical Society's journal Nano Letters.

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Enrique Gomez, assistant professor of chemical engineering, can be contacted at edg12@psu.edu. For more information, read the news release by Curtis Chan on the MRINews Page:

http://www.mri.psu.edu/news/ or watch the video.

Work by a research team at Penn State and Rice University could lead to the development of flexible solar cells. The engineers' technique centers on control of the nanostructure and morphology to create organic solar cells made of block polymers. Credit: Curtis Chan, Penn State



MICROENCAPSULATION PRODUCES UNIFORM **DRUG RELEASE VEHICLE**



Scanning electron micrograph of BCNU-loaded microspheres (black and white background) with 3d rendered images of brain cancers cells (yellow) and released BCNU (purple). Credit: Abidian Lab

A new method of delivering anticancer drugs directly to tumors of the brain is being developed by researchers in biomedical and chemical engineering. By encapsulating the drug BCNU in FDA-approved biodegradable polymer microspheres, the drugs can be safely injected into the tumor where they can be controllably released over time. The encapsulation of the drug avoids the side effects from intravenous chemotherapy, which can affect the whole body. Another method that leaves a drug infused wafer in the tumor after surgery requires another surgery when the drug runs out. Researchers Mohammad Reza Abidian, Pouria Fattahi, and Ali Borhan, used a low cost electrojetting process to make the spheres, which can be used to deliver other types of drugs as well.

Mohammad Abidian, assistant professor of biomedical engineering, chemical engineering, and materials science and engineering, can be contacted at mabidian@engr.psu.edu. Read the news release by A'ndrea Elyse Messer on the MRI News Page: http://www.mri.psu.edu/news/.

GENOME OF ELASTOMERIC MATERIALS CREATES NOVEL MATERIALS

Melik Demirel, professor of engineering science and mechanics, was part of an international team looking to produce unique materials based on biological templates. The specimens studied included the egg case membranes of a tropical marine snail with unusual shock-absorbing properties and elasticity; mussel foot with self-healing properties; and squid teeth with a nanotube structure of strong polymers. "We now know that nature can do all kinds of things including nanotubes, cross-linked structures and shock-absorbing coils," said Demirel. "Now that we know the secrets, we need to find ways to mimic the structures and do it inexpensively." Their work, supported in part by the Office of Naval Research and NIH, was published in Nature Biotechnology.

Melik Demirel can be contacted at mdemirel@engr.psu.edu. Read the news release by A'ndrea Elyse Messer on the MRI News Page: http://www.mri.psu.edu/news/.

TINY FILTER SCREENS OUT CANCER CELLS



This tiny mesh structure is designed to capture tumor cells. Credit: College of Engineering, Penn State



Melik C.Demirel holds a squid used in biomimetic materials research Credit: Demirel Lab

Circulating tumor cells (CTCs) in the blood are the culprits behind metastasis, the spread of cancer to other organs in the body. Siyang Zheng and his research group in biomedical engineering have developed a small filter that can capture CTCs while preserving their viability. Called a flexible micro spring array, the device is highly porous, flexible, and requires low driving pressure to push the blood through the mesh of tiny s-shaped filters. By capturing the tumor cells, it will be possible to monitor cancer treatment and modify it if necessary.

Siyang Zheng is assistant professor of bioengineering. He can be reached at siyang@psu.edu. For more information, read the news release by Curtis Chan on the MRINews Page: http://www.mri.psu.edu/news/.

LASER TECHNIQUE ENABLES 3D ANALYSIS AND NATURAL COLOR IMAGES



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Laser tomography 3D view of a Yellowjacket bead

Internal structure of a maize root

A new technology invented to automate the laborious process of preparing plant roots for phenotyping has morphed into a powerful tool for exploring the three-dimensional structure of small objects. Now, two former Penn State students have formed a startup company targeting agribusiness and horticultural research.



Ben Hall (L) and Brian Reinhardt in the L4IS office at Innovation Park

The standard method of preparing root samples for analysis requires cutting thin slices of root by hand, a

process that yields four to five slices per hour. Jonathan Lynch, a professor of plant nutrition at Penn State and head of the Roots Lab, had a backlog of 20,000 samples he was studying to improve drought tolerance and nutritional uptake in low fertility soil. Benjamin Hall was an undergraduate student in energy engineering working parttime in the laser lab of the Applied

Research Laboratory at Penn State.



A cicada is laser ablated and digitally reconstructed using 3D imaging software.

Lynch applied for a small grant from the National Science Foundation's Research Experience for Undergraduates (REU) program, which funded Hall to work on a project to apply lasers for slicing his root samples. Using a nanosecond-pulse laser, Hall developed a method to slice 11 identically spaced root samples per second. (The Lie bigst characteristic structure) and the state of th

Using a nanosecond-pulse laser, Hall developed a method to slice 11 identically spaced root samples per second. "Then I had to take the samples all the way across campus to the root lab to have them analyzed," Hall says. "It was easier to buy a good camera lens and take the photos myself and send the files to the lab."

At a recent talk at Penn State's Millennium Science "It was easier to buy a good camera lens and take the Complex, Hall wowed the audience with images of the photos myself and send the files to the lab." complex internal structures of plants and insects. But beyond the wow factor, it was the possibility of gathering Hall struggled with finding the proper backlighting to scientific data in a colorful, clear, and detailed threemake clear images but eventually discovered that the laser dimensional representation that had the audience talking. itself provided sufficient light to light up the image while it There were suggestions for new scientific uses for his was being cut. By placing the root on a moveable platform technology, which Hall welcomed. "We don't even know beneath the laser, he could incrementally vaporize sections what all we can do with this yet. of the root, leaving a series of clear surface images, which could be combined with software to make a 3D rendering "Technology is moving so fast. There are techniques we of the interior and exterior of the sample.

"This is a tomography technique, and there are others out there," says Hall. "But X-ray tomography basically works by mapping the density of a substance, which is great unless the specimen has different materials of similar density. That can make it hard to differentiate structures, so it can be difficult to quantify measurements. Magnetic resonance imaging (MRI) we're not even competing with. Those machines are so big and complex, and so expensive to operate compared to our system."

The laser tomography method is novel in that it provides high contrast, full color images without the use of

contrast enhancing agents. This allows researchers to see nuanced compositional differences in their samples they

would not be able to see otherwise. Additional benefits of the laser tomography method are its speed, on the order of minutes, and that in most cases no preparation is required for the small biological specimens studied.

Penn State has applied for a patent, and Hall and his business partner Brian Reinhardt, a former Penn State graduate student, have

"Technology is moving so fast. There are techniques we can combine with ours to get chemical information out of the samples. We have to start approaching some of these scientific problems differently. We can do 3D analysis. Now what else can we do?"

Included on the patent are Hall and his Penn State advisers, Jonathan Lynch and Ted Reutzel. Hall is currently working with Lynch on a paper describing their method. Ben Franklin Technology Partners of Central and Northern Pennsylvania provided funding and business assistance to start the company, and the Ben Franklin TechCelerator @ State College provided valuable entrepreneurial training. Visit the L4IS website at http://l4is.com. To view videos of their laser tomography, go to http://www.youtube.com/user/L4ISLLC. Contact Benjamin Hall at hall.benjamin@gmail.com.



Difference Engine No.2 in the Computer History Museum. Credit: Marcin Wichary, Wikimedia

room and proved too expensive to complete, even for its financier, the British government. According to An Illustrated History of Computers (2002), the first computer programmer was Ada Byron, 19-year-old daughter of Lord Byron. Fascinated by Babbage's creation, Ada wrote a series of instructions for another Babbage invention, the Analytic Engine, also unbuilt.

In the 1940s, the first electro-mechanical computer was built in a collaboration between IBM and Harvard. The five-ton, 51-foot-long Harvard Mark 1 was capable of storing only 72 numbers in its memory. Penn State was one of the first universities to build its own computer for research, the PENNSTAC, Penn State Automatic Computer, in 1956. By 1962, there was still only one large computer for the entire campus, with only 10KB of memory. Today, Penn State's Research Computing and Cyberinfrastructure Group oversees 17 computing clusters with over 12,000 processor cores. Students and faculty gain access to the clusters from their desktop or laptop computers to do calculations that just a few years ago would have taken months to complete, if they could have been done at all.

The Penn State Institute for CyberScience, a university-wide interdisciplinary unit under the direction of institute director Padma Raghavan, has embarked on a transformative program to enable computation and data-enabled science and engineering across the university. This includes the hiring of a dozen new faculty who can work across disciplines on large data mining and simulation projects in fields such as bioinformatics, astrophysics, geosciences, and high throughput materials discovery. By adding a world-class computational component to Penn State's core disciplinary strengths, Penn State will become even more successful at competing for large scale federal grants, such as the recent \$10 million Expeditions in Computing award described in this issue.

PDATING THE DIFFERENCE ENGINE

Inventors have been fascinated by calculating machines for centuries. Leonardo made drawings of gears to be used for computing. The young Blaise Pascal invented the mechanical calculator in 1642 to help his father, a tax collector. The first punch card calculator was invented by a Frenchman in 1801. And Englishman Charles Babbage invented his famous steam-driven calculating machine, called the Difference Engine, in the 1820s, in order to improve on the manual calculations in the British navigation tables. The Difference Engine was a contraption of gears and cogs the size of a

In materials research alone, Penn State has dozens of research groups who use modeling and simulation as a component of their study of advanced materials and materials processing. Some of those modeling methods were developed on this campus. Penn State is also pioneering new types of computer architecture, new hardware, and going beyond silicon to make smarter, faster, more energy efficient computers. In this issue, we introduce a handful of Penn State's materials researchers who are at work on computing for the future.

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Energy Solutions Using Atomic Scale Modeling

Only around 9 percent of our energy consumption in the U.S. comes from renewables, of which only 13 percent is from wind and less than 2 percent from solar. Growth in the use of wind and solar energy is hobbled due to the well-known problem of intermittency; that is, wind and sun are not always available when the need for them is greatest. Advances in energy storage technologies are crucial to making renewable energy a larger share of the energy mix. Materials scientists and engineers at Penn State are building experimental batteries and fuel cells, but it is not always easy to know what exactly is happening inside these devices, especially at the level of the charged atoms and electrons that create current.

Ismaila Dabo, a new assistant professor of materials science and engineering, wants to use quantum simulations and multiscale modeling to understand the complex interactions inside those energy storage devices when experimental probes fail. Using a wellestablished technique called density functional theory and open source software he is helping to develop called Quantum Espresso, Dabo hopes to bring more clarity to the internal environment of fuel cells and batteries, thereby helping his experimentalist colleagues make energy storage more efficient and less costly.

Dabo arrived on campus this summer from Ecole des Ponts ParisTech, the engineering school of the University of Paris-Est, where he was a post-doc and then a permanent researcher in the Department of Scientific Computing. Dabo did his doctoral work under Nicola Marzari at MIT, where he did research on chemical poisoning in low-temperature fuel cells and developed computational tools to study quantum

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systems in electrochemical environments. As he begins building his own research program, he will join a group of faculty members who are developing advanced computational materials design tools, along with the experimentalists who are benefitting from their work. "It's amazing how many opportunities there are for collaboration here," Dabo remarked. "Maybe being at Penn State you don't realize that, but coming from the outside, it's one of the specificities of this university."

Dabo's intends to understand precisely what is happening in batteries when they deliver current. As an example, he points to the battery in a cell phone, which is composed of stacked layers of materials that conduct charged particles – either electrons or ions. Dabo's simulations, based on quantum theory, predict the flow of charged particles at the interface of those layers of materials. It is at the interface, he says, where many of the battery limitations occur. To understand the complex physical and chemical environment within the battery, Dabo turns to multiscale models. Whereas most quantum simulation approaches model atoms as discrete nuclei surrounded by a cloud of electrons, multiscale approaches model groups of atoms up to continuous masses. The chemical reactions in a battery take place on the scale of atoms, whereas voltage is a macroscale quantity, something that can be measured at the human scale. Multiscale modeling attempts to bridge these disparate size scales in order to, for example, explain how chemical reactions result in voltage.

Quantum Espresso is one of the tools he and many other modelers are developing to achieve better precision in making quantum mechanical calculations and applying them to macroscale effects such as voltage, temperature, and pressure. "Quantum Espresso is on the atomic level, but there is work to include the multiscale, and my group participates in this effort," Dabo said. "It's a multiuniversity multi-collaborator effort."

Simplify, simplify

Even with the big computers now available to researchers, computing at the atomic level is costly. For larger calculations, computer clusters with up to several thousand cores are required, and may take from a day up to several months of computation time to do complex calculations. Dabo explained that in order to store the three dimensional wave function that

represents one electron, a 3D grid is created with each point in the grid located by three data points. If the grid resolution is of 100 points along each direction, that guickly adds up to one million points of data that must be stored. Add in more electrons and the number of data points rapidly explodes. The interactions between all of these bits need to be simplified to make the calculations feasible.

In quantum mechanics, Dabo continued, the fundamental equation is the Schrödinger equation, which explains the interactions between electrons. Erwin Schrödinger, one of the foundational figures in developing quantum theory, wrote the equations that described the wave mechanics of electrons, and formulated the famous Schrödinger's Cat paradox*.

"All the electrons interact with one another," Dabo explained. "You really need to understand where all the electrons sit to correctly describe the state of the system." To simplify these complex interactions, physicists and chemists often use a modeling method developed in the last decades of the 20th century called density functional theory. In this method, you don't take into account the interactions of each electron with all the others. Instead, the interaction of one electron with the crowd of other electrons is accounted for, and that interaction is related to electron density in space. This replaces a complex many-body problem with a much simpler one-body problem.

Still, there are limitations to the theory and understanding what happens in materials at the atom level is extremely complicated. This is where interacting with experimentalists is helpful, Dabo remarked. Advances in microscopy and spectroscopy make it possible to obtain data at the atomic scale. Microscop such as the FEI Titan³ scanning/transmission electro microscope in MRI's Materials Characterization Lab can look at atoms and map their locations at the sub-Angstrom level, while spectroscopy techniques (also available in MCL) send light or other types of radiati at a material to see how the material reacts. Both experimental techniques are providing better time an space resolution to researchers. Yet at the same time, the experimental data are becoming more complicated Dabo said that by using quantum mechanics to predict the outcome of experiments beforehand, then comparing the experiments to the model, if the two results match, it is possible to go back and look at the details of the calculation and see what really happene with the atoms and electrons.

The Materials Genome Project

"Materials science is at the frontier between physics, Ismaila Dabo is assistant professor of materials science chemistry, and even computer science," Dabo reflected. and engineering. Contact him at dabo@matse.psu.edu. "A lot of the problems we have to face at the technology level come down to improving materials."

The Materials Genome Initiative announced by the White House in June 2011 is the federal government's



* Schrödinger's Cat

In Erwin Schrödinger's well-known thought experiment, a cat is placed in a box with a Geiger counter, a radioactive sample, and a bottle of poison. If the Geiger counter detects that the sample has decayed, it will break the bottle and release the poison. One version of quantum theory says that until the box is opened, the random event of the emission of a subatomic particle is in superposition both having occurred and not occurred. Schrödinger was pointing out that this would require the cat to be both alive and dead until the box was opened, which he considered absurd. However, quantum superposition, the theory that grew out of the Schrödinger equation, is the basis for quantum computing.

"Quantum ESPRESSO is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

Quantum ESPRESSO has evolved into a distribution of independent and inter-operable codes in the spirit of an open-source project. The Quantum ESPRESSO distribution

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	plan to accelerate the process of developing new
nic	materials and processes by making information
ng	freely available to researchers and entrepreneurs.
	It is generally acknowledged that a new material
	can take as much as 20 years to reach market. "The
bes,	initiative will fund computational tools, software,
on	new methods for material characterization, and the
)	development of open standards and databases that
	will make the process of discovery and development
	of advanced materials faster, less expensive, and more
ion	predictable," according to the Office of Science and
	Technology Policy announcement.
nd	
	With a goal of accelerating discovery in materials
d	in a way similar to the Human Genome Project's
	acceleration of biological sciences, the Materials
	Genome Initiative will screen tens of thousands of
L	chemical compositions computationally to predict their
	main properties for any desired application. "When
, 	you have 1000 materials, you cannot study them all
ea	experimentally." Dabo said. "Based on computation.
	you may reduce this to 10 materials that you than
	you may reduce this to to materials that you then
	study experimentally."

consists of a "historical" core set of components, and a
set of plug-ins that perform more advanced tasks, plus
a number of third-party packages designed to be inter-
operable with the core components. Researchers active
in the field of electronic-structure calculations are
encouraged to participate in the project by contributing
their own codes or by implementing their own ideas into
existing codes." — From www.quantum-espresso.org

A QUANTUM ESPRESSO WORKSHOP will be held at Penn State University June 16-20, 2014. For information, visit their website at msc.psu.edu/qe2014.

LONG-OING CHEN: MODELER ATTHE MESOSCALE

Modeling at the electronic/ atomic scale based on quantum mechanics has been very successful in predicting the properties of new materials systems, but there are limitations.

Most of the calculations based on density functional theory are performed assuming a temperature of zero Kelvin and assuming a perfect crystal structure. And even really large computers can model only a few hundreds of atoms over a very brief time scale measured in picoseconds. We can increase the system size in atomic scale simulations to millions of atoms by using more approximate descriptions of interatomic interactions among atoms called empirical potentials. However, the sizes are still too small compared to most structures of interest in practical materials systems, such as the aluminum alloys used in automobiles and nickel alloys in turbine engines in which millions of nanoscale precipitate particles give them useful properties. Anything that changes over a large volume and a relatively long time, e.g., minutes or hours, cannot really be modeled atomically.

Modeling microstructures

Long-Qing Chen, distinguished professor of materials science and engineering, works at a larger scale developing modeling techniques to predict features called microstructures. Microstructure refers to the mesoscale features that are intermediate in size between the nanoscale and bulk scale and can include grains of different shapes and sizes, different phases or crystal structures, different electrical or magnetic polarization, and various defects. These features are what determine the mechanical, electrical, magnetic, and optical properties of a material, according to Chen. Therefore, we achieve the desired properties by controlling microstructures.

Chen is widely known among materials scientists for developing solutions to modeling at the

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mesoscale using a technique called phase-field modeling. "The phase-field approach is perhaps the most powerful approach for predicting microstructure evolution under different processing conditions with different compositions as a function of time," Chen says.

What is phase-field modeling?

"We used to model the interface motion by assuming a sharp mathematical interface between two different materials," Chen remarks. "We thought the material on one side would behave in one way and that on the other side of the interface it would behave differently. Then at the interface you would somehow have to define some kind of boundary conditions."

Phase-field, however, assumes there is a gradual change from one material to another. The interface is smoothed out. This is not a new idea, says Chen, having been proposed by Dutch scientist Johannes van der Waals more than a century ago. But phasefield models really took off in the 1990s when two researchers, a mathematician and a physicist, tried to model the dendrite growth during solidification of a liquid. Since then it has been applied to many areas, including phase transformations in alloys, crystal growth in vapor deposition, grain growth, ferroelectric materials, topological optimization, and image processing.

Chen has also applied phase-field equations to a variety of materials applications: alloy microstructures, ferroelectric domain microstructures, capacitor degradation, and battery or solid oxide fuel cell electrode microstructures.

Some of the phase-field models proposed by Chen's group have been picked up by other computational groups. "It's nice to see other people utilizing what we proposed," he says. "Examples include phase-field models for grain growth, precipitate microstructures in alloys, and domain structures in ferroelectric materials."

Working with experimentalists

The Chen group uses phase-field techniques

to help experimental groups at Penn State and other universities, as well as industry partners who are developing new alloys for automotive and aerospace, to design and control microstructure. "One of the features of our group is our work with experimentalists," Chen says. "We work with more than a dozen experimental groups, many in the area of oxide ferroelectric and multiferroic thin films."

Oxide ferroelectric thin films are used in applications as diverse as piezoelectric actuators, ferroelectric memory, etc. Multiferroics are materials with both ferroelectric and ferromagnetic properties. Ferroelectric materials have a permanent electric polarization that can be reversed by an external electric field. Ferromagnetic materials can be given magnetic properties by applying an external magnetic field. Chen's group helps experimentalists figure out how to produce particular domain structures in thin films by choosing different substrates, processing at different temperatures, or applying fields.

"Doing experiments, it is very difficult to get into the details of the physical mechanisms underlying the phenomenon that you observe. But using simulation, we can get at all the details of what's happening inside a material. A lot of times it can really help experimentalists understand what they've observed or measured," Chen says.

"Our collaborations with experimental groups have led to many joint publications. My students communicate with students in experimental groups, and sometimes we can even provide predictions and guidance to experiments," he continues.

For example, classic lead-free materials such as BaTiO₃ and KNbO₃ undergo a series of ferroelectric transitions upon heating, sequentially adopting rhombohedral, orthorhombic, and tetragonal ferroelectric phases before reverting to the cubic parent phase in a single crystal single domain state. In multi-domain configurations however, his phasefield simulations predict the emergence of a new phase of monoclinic symmetry, thermodynamically stabilized in significant volume fractions (20-60%)



Predicted crystal domain structure of a ferroelectric material Credit: L-Q Chen, Penn State

over a wide temperature range of over 100 K. The figure shows an example of predicted domain structure consisting of several phases including the new monoclinic phases represented in different colors. Such a new phase was experimentally confirmed by Professor Gopalan's group at Penn State using a nonlinear optical Second Harmonic Generation (SHG) imaging technique.

In the future, if funding arrives, Chen could be working with battery experts at Penn State to try to solve one of the grand challenges in energy related research, which is to dramatically improve the solid electrolyte materials for batteries. He is currently involved in a GOALI (Grant Opportunities for Academic Liaison with Industry) program in collaboration with General Motors to study dendrite growth during battery charging and in a NETL project on modeling degradation of electrode microstructures in solid oxide fuel cells.

Long-Qing Chen is a fellow of the Materials Research Society and American Physical Society, and received a Guggenheim Fellowship in 2005-2006, in addition to many other awards. His publications have been cited over 12,000 times. He can be contacted at lqc3@psu.edu.



Beyond Silicon: Transistors for the Future

It has been over 60 years since the transistor was invented at Bell Labs. Since that time, the workhorse of the computer age has shrunk from the size of a baseball to the point where more than 60 million 2 nm transistors could fit onto the head of a pin, according to an Intel white paper. Bell Labs' first transistor used germanium as the semiconductor, but germanium was difficult to purify and hard to manufacture. By 1954, Bell Labs had produced the first silicon transistors, and the race was on.

To most Americans at the beginning of the silicon age in the 1950s and early 1960s, a

transistor was something akin to a pocket radio you took to the beach to listen to surf music and the Beatles. Computers still filled an entire room and were meant for scientists only. That same Intel paper compares their first microprocessor, introduced in 1971, to recent versions at 32 nm and finds that processor is 4000 times as fast and uses 4000 times less energy. By 2014, Intel expects to begin producing at the 14 nm node, which means that the channel length of the transistor is less than 30 atoms across.

Suman Datta, professor of electrical engineering, spent eight years in the Advanced Transistor Research Group at Intel, in Hillsboro, Oregon, helping to introduce a strained channel silicon transistor technology that went into products at the 130 nm as well as the current 20 nm nodes. Another breakthrough came when his group at Intel found a replacement for silicon dioxide, the standard dielectric in the CMOS 000



transistor, with a transition metal oxide that allowed scaling to continue. The thickness of the gate dielectric had shrunk so much that with silicon dioxide they had only three layers of atoms left; they had literally run out of atoms. "At that point in time, scaling would have come to a screeching halt," Datta says. But by swapping out the silicon dioxide for a transition metal oxide with a higher dielectric constant, they could resume scaling and miniaturization of transistors. Gordon Moore, co-founder of Intel and the author of the observation called Moore's Law that transistors would drop in size and prices fall correspondingly about every 18 months, emailed the group to congratulate them when the breakthrough was announced, calling it the biggest change in transistor technology since the invention of the transistor at Bell Labs.

Datta was also involved in another big change in transistor technology, the first change from a planar, or flat, architecture to a non-planar or 3D architecture. It was planar technology developed in the 1970s that allowed the first integrated circuits to be built. But as the active parts of the transistor got closer together, current began to flow from the source to the drain even in the off-state. Called leakage current, it could drain the battery in a laptop or cell phone even when they were not

in use. They decided they could overcome this problem by making multiple gates to control the flow of current instead of the one gate in planar devices. To do this they flipped the transistor on its side, creating what looked like a fin. This geometry allowed them to wrap the gate around the three sides of the fin. The 3D technology is now in the latest microprocessors used in high-end laptops, desktops, and data centers.

More of Moore

In 2007, Datta left Intel and joined Penn State's Department of Electrical Engineering to work on more high risk transistor projects, hoping to stay ahead of the technology and possibly lay the groundwork for future transistor and microchip technologies. Penn State's materials expertise intrigued him, because he wanted to see if he could incorporate more exotic non-silicon materials into a device that could still be incorporated into the familiar CMOS architecture.

"If you go to a store today, you don't necessarily get microprocessors with faster clock speed," Datta remarks. "What people are looking for is energy efficiency. Can we provide more performance per watt of energy that these transistors consume by using an exotic material such as compound semiconductors?"



A lattice of uncompressed Germanium atoms on a Silicon Germanium buffer Epitaxial growth compresses the Germanium layer, providing improved electronic properties.

Credit all: Datta group



quantum well MOSFET with a 1 nm Silicon cap and 1 nm Aluminum oxide/4 nm Hafnium oxide dielectric



A scanning electron microscope top view of a tunneling field effect transistor Credit: Datta group

That is one of the challenges he and his students have been tackling in Penn State's Nanofabrication Laboratory cleanroom – building a prototype transistor that can operate on lower voltage than standard CMOS devices yet maintain high performance and power efficiency. They have made substantial progress.

At the International Electron Devices Meeting in December, 2013, Datta's graduate student Bijesh Rajamohanan, presented a paper on a highfrequency, low-power tunneling transistor that could deliver high performance at about half the voltage of standard silicon transistors. Tunnel field effect transistors are considered to be a potential replacement for current CMOS transistors, as device makers search for a way to continue shrinking the size of transistors and packing more transistors into a given area - Moore's Law. Tunneling is a quantum effect in which electrons are able to cross through a potential barrier, in this case an extremely thin interface between the source and the channel. The researchers tuned the material composition of the indium gallium arsenide/gallium arsenide antimony so that the energy barrier was close to zero, which allowed electrons to tunnel through the barrier when desired. To improve amplification, the researchers moved all the contacts to the same plane at the top

Professor Suman Datta leads the Nanoelectronics Devices and Circuits Lab http://www.ndcl.ee.psu.edu/

surface of the vertical transistor. The researchers from National Institute for Standards and Testing (NIST) and custom wafer manufacturer IQE Inc. were co-presenters.

More than Moore

Another direction his group is following is one that he calls "More than Moore," which means that in the next generation of applications in information technology, people will be interested in interacting more directly with their computer. Called proactive or perceptual computing, this technology would go beyond the keyboard and mouse by creating user-machine interfaces that were not traditionally a part of Moore's Law. Datta's group is looking at sensitive microelectromechanical systems (MEMS)-based magnetic sensors directly integrated with CMOS technology that could record and interpret brain signals, possibly allowing a person one day to compose an email with her thoughts.

This sounds well into the realm of fantasy; however, Datta says that Microsoft, Samsung, Intel, Google, and several other companies are strongly pursuing perceptual computing.

Beyond Moore

The third area they are involved in takes them beyond the traditional realms of computing into



an area they call "Beyond Moore." Traditional computing is still done using ones and zeroes – digital bits. The brain, however, works differently, Datta explains. "When I see you, I immediately know who you are, where I've seen you, what is the context, why we are here. That is done through a very different computing paradigm that Mother Nature has figured out over many millions of years of evolution. So, one of the areas that we are moving strongly into is to try to see whether, with artificial hardware, we can implement what we call this neuromorphic computing paradigm where we don't do things with ones and zeroes, but do them in an associative sense."

The direction in which this device research is leading in Datta's group is toward coupled oscillators using complex oxide materials. There is a phenomenon called biological synchronization in which two weakly coupled oscillators will go into resonance when a certain set of patterns is presented to the oscillators. This ability to couple the oscillators' relative frequency and phase to a pattern could have implications for neuromorphic pattern recognition, for example machine vision. Datta is part of a large team of researchers looking into implementing vision algorithms on new types of hardware. (See the following article "An Expedition in Computing Team Forms to Create a Cognitive Camera".)

"We are interested in taking advantage of the complex oxide expertise resident at Penn State to try to build these novel devices that go beyond just Boolean computing. It's a new paradigm of computation that folks are very interested in," says Datta.

Innovate to survive

Datta brings his research experience in industry into the classroom and the lab. He believes that in order to sustain innovation, his students need to have a strong grasp of the fundamentals in physics, chemistry, and mathematics. "Students lose interest and want to know why they can't skip through the mathematical equations and start building and testing stuff. Because of my unique background at Intel R&D, I can tell them that without mastering the equations I learned as a student I would not have been able to make these contributions later on. I help students understand that we are in the high-tech world where innovation is the only way you survive. Or else you become extinct like the dinosaurs."

Suman Datta, professor of electrical engineering, was part of the Intel team awarded the 2012 SEMI Award for North America for the invention of the high-k plus metal gate transistor. The award is the highest honor conferred by the 2,000 member global industry association for the semiconductor industry. Professor Datta can be contacted at sdatta@engr.psu.edu.

PENNSTATE PENN STATE PLAYS PROMINENT ROLE IN TWO NEW CENTERS

Penn State faculty lead two of the four research themes in the LEAST Center, the Center for Low Energy Systems Technology, a consortium of 10 universities, led by Notre Dame, funded by DARPA and the Semiconductor Research Corporation to explore new concepts for dramatically lowering the power requirements for electronics. Visit the LEAST website at **least.nd.edu**.

Penn State and MRI also play a major role in the ASSIST Center, an NSF Nanosystems Engineering Research Center for Advanced Self-powered Systems of Integrated Sensors and Technologies, led by North Carolina State University. Penn State faculty lead two of the five technical thrusts as well as acting as the Research Director for the five-year \$18.5 million project. Visit the ASSIST website at **assist.ncsu.edu**. AN EXPEDITION IN COMPUTING TEAM FORMS TO CREATE A COGNITIVE CAMERA

Penn State researchers, along with colleagues around the U.S., are embarking on a scientific voyage of discovery, an expedition to recreate the human visual system on a computer chip. This particular undertaking is sponsored by the National Science Foundation's Directorate for Computer and Information Science and Engineering (CISE). Called the Expedition in Computing program, it is one of the largest investments in computer science that the National Science Foundation makes, according to the principal investigator, Penn State professor of computer science and electrical engineering Vijaykrishnan Narayanan.



A camera with on-board computational power for intelligent video processing

Narayanan leads a distinguished team of researchers from eight universities, in collaborations with national labs, and industry. Inspired by biological vision, and particularly the human visual cortex, the multidisciplinary team will try to far surpass current vision technology to build what they are calling a smart or cognitive camera. These machine vision systems will understand and interact with their surroundings, intelligently analyze complex scenes, and interact with their users. The project builds on five years of previous work on smart camera systems in which Narayanan collaborated with the University of Southern California and MIT.

Calling their project Visual Cortex on Silicon, the multidisciplinary team will attempt to understand how the human visual cortex works and to turn that knowledge into computer vision algorithms. Other

team members will design new types of computing architecture based on CMOS and beyond-CMOS technologies to support these vision algorithms. The brain has enormous connectivity, with the memory and compute features built together. Suman Datta, a Penn State professor of electrical engineering, and

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of the Visual Cortex on Silicon project is to approach and eventually exceed the efficiency of human vision.

Applications of a cognitive camera

The applications for a smart camera that can process information and make decisions are many, ranging



Vijay Narayanan (holding camera) and his graduate students involved with the design of smart camera systems

Philip Wong of Stanford University will build dense analog memory devices similar to the brain's synapse/ neuron architecture using new materials systems. Finally, team members from Penn State will integrate the vision system into low-power electronic devices that interface with human beings.

Current machine vision systems are usually large, power hungry, and designed for one specific application, such as the face recognition feature found in many digital cameras. On the other hand, the human visual cortex is a multipurpose instrument, capable of making sense out of highly cluttered environments and accomplishing a range of visual tasks while consuming less than 20 Watts of power. Current vision systems can recognize around 20 distinct object classes. Narayanan and his team want to increase that number to 100 or more, especially in cluttered environments such as city streets. The goal

from the simple, such as warning distracted drivers when they have taken their eyes off the road for too long, to the complex, for instance, recognizing a potential terrorist attack such as the Boston Marathon massacre or the London underground train bombings.

Distracted driving is responsible for well over a quarter million injuries each year and more than 3,000 fatalities. A driver attention system, because of its capability to reduce serious accidents, will be one of several priorities

for the Visual Cortex on Silicon team. "We will also be working to draw a driver's attention to things in the environment they might have missed," Narayanan explains.

A second research priority will be to assist the visually impaired. As the population ages, vision impairment becomes a larger societal problem. A goal is to build low-power devices that can replicate the human vision system in a wearable form. Unlike Google glass, which has limited on-board intelligence and must connect to the "cloud" in order to compute, the system Narayanan and colleagues envision will have embedded computation. "Communication via the cloud is always quite expensive and can be a significant drain on battery life," says Narayanan. "There are also applications and situations where connectivity is not available or too slow." Speed can be crucial when a sightimpaired person is attempting to navigate a busy street.

Less societally significant, perhaps, but even more universal, a wearable smart camera will enhance reality in retail shopping and travel, doing calculations to compare prices, providing consumer information, or providing travel commentary about local landmarks. It will be like having a tour guide with you on your trip, Narayanan says.

The need for public safety versus the need for privacy is a controversial topic, and the researchers are sensitive to the issue and intend to address it.

Cognitive cameras with the ability to recognize unusual behavior and alert authorities will make decisions about where and how such systems should be used more timely than ever. "We have people in our group who will give us insight into the social ramifications of our technology," Narayanan says optimistically. "Before Boston, people were saying cameras were spying on us. How do we ensure that people who need this are not bothered by it?"

The program has large implication, both societally and scientifically. Much is already understood about how the human visual cortex works, and the bottomup camera technology, beginning with raw pixels, is



very advanced. The top-down workings of a machine vision system will be the challenge - for instance, what is the difference between a person blind from birth and one who was recently blinded? How are we influenced in that case by what we already know, shapes and colors and perspective? How do we orient ourselves in space? These are not trivial considerations. Scientifically, the project is expected to develop interesting new algorithms that may tell us more about how the brain operates; create models that will help to better explain the visual cortex; design new computing architecture and a customized routing structure; develop integrated computing and memory for energy efficiency; and design human/ machine interfaces.

"With this large Expeditions in Computing award, we have been able to put together a team of top researchers from across the country and across disciplines. This cross-disciplinarity is making us attractive to top people outside Penn State. We have many champions in different areas. It's huge for our students and good for research," Narayanan concludes.

Vijay Narayanan is professor of computer science and engineering and electrical engineering at Penn State and co-director of the Microsystems Design lab. Contact him at vijay@cse.psu.edu.

Graduate student Yang Xiao demonstrates a camera that recognizes objects and displays them on a screen, with a bounding box and name of the object.

Connecting Transistors:

A Problem in Scaling

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One of the limiting factors in the ongoing shrinking of components in computer chip technology is the problem of interconnects, the wires that carry power into, across, and between integrated circuits. The Suzanne Mohney group at Penn State is expert in the electronic properties of materials and in understanding the reactions between metal and semiconductor contacts in microelectronics. This work on interconnects is new to her group, but it builds on past work on thin films for MEMS, and on wide expertise in deposition, lithography, and electrical characterization.

> Ph.D. student Anna Domask works on interconnects in the Mohney group.



silver wires which connect the die to legs of the chip. Credit: Zephyris (Richard Wheeler) and the English language Wikipedia

Interconnects have been important ever since the first integrated circuit was developed in the 1950s and its transistors needed a way to get and discharge current. Interconnects are the tiny "wires" that connect individual transistors or connect one area of a microchip with another area. They can be relatively large, when connecting to the power coming into the microchip, or extremely small, when connecting two transistors. In the early 2000s, the material of choice for these wires moved from aluminum to copper, the current standard. But as the size of the wires grows ever smaller, problems arise with copper as the material for carrying current.

Anna Domask, a Ph.D. student in Mohney's group, is working to find new materials to help solve the interconnect-scalability problem for the next generation of devices. The problem with interconnects, she says, is electromigration.

An EPROM microchip die showing the detail of the integrated circuit itself and the

Electromigration is the wholesale diffusion of atoms within these tiny wires due to the transfer of momentum from electrons to metal atoms. This diffusion creates void spaces called valleys, through which no current can pass, or hillocks, where the wire bulges out and can touch another wire, causing a short circuit.

As with many other material effects, electromigration becomes a larger problem as length scales shrink. "Intel just released its 14 nm chip with a 14 nm gate length. With smaller chips, you need smaller wires to get power to adjacent transistors. As the interconnects between transistors shrink, the effects of electromigration get worse as the current density increases, which it does as the inverse square of the wire diameter," Domask explains. If you halve the diameter, the current density increases by a factor of four.

The problem with copper, which is one of technology's most conductive materials, is that at small dimensions resistivity increases dramatically. In addition to the increased power density, wires that are only 10 nm across see a dramatic increase in electron scattering due to surface and grain boundary effects caused by increased surface-to-volume ratio and the decreased grain sizes. Copper is especially susceptible to electromigration because it is a soft, FCC (face-centered cubic) metal that readily self-diffuses.

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For these reasons, copper interconnects have become one of the barriers to the continued scaling of microchips. Many groups around the world are looking for ways around the problems of electromigration and increasing wire resistance. Some groups are looking at metals that have higher bulk resistivity but could potentially perform better than copper at small diameters. That might be a possible solution for the near future, because existing manufacturing processes could be used. Other groups are looking at intermetallic systems, nickel silicide in particular, because they are harder and less selfdiffusive. Lastly, some groups are looking at carbon nanotubes and other nano-structures, which would be a longer-term solution if scientists could learn to manufacture them on an industrial scale and incorporate them into the industrial processes used to make microelectronic devices. Because carbon nanotubes are already scaled to an appropriate size for interconnects, and have extremely low resistivity due to their hexagonal crystal structure, they have been used successfully to connect various devices in the laboratory. Unfortunately, currently they must be placed individually, which is not viable for mass production. Graphene, another material being considered, has many of the same manufacturability problems as carbon nanotubes.

The Penn State group is looking at different intermetallic systems, trying to find the right balance between bulk resistivity and electromigration susceptibility. The particular intermetallic systems they are looking at have not been studied extensively at the small scale they are interested in. Along with controlling materials properties, they must engineer

the surfaces to be as pristine as possible. "Due to their geometry, the wires are going to have a lot of surface," Domask notes. "We know surface roughness and surface contamination increase resistivity, so we must control both of those factors in our experiments." Incorporating a new material into a well-developed technology such as microprocessors has multiple challenges. Researchers need to understand how any new materials will interact with the other materials in the device, such as silicon dioxide, or high- κ dielectrics such as hafnium oxide. It's not the same as running a copper wire in your house, says Domask. "It's not just understanding the scale of the material, but how you get it into a large integrated device and then make it manufacturable." The earlier move from aluminum to copper had a fringe benefit: it eliminated a manufacturing step. Whatever new material the semiconductor industry chooses to adopt, manufacturability and industrial scalability will be almost as important as any material's property.

The new Millennium Science Complex's interdisciplinary open environment greatly improved collaboration between Domask and students in other departments working on closely related projects. Her group's expertise in materials characterization and the science of materials complements the work of Suman Datta's students, for example. Datta's students bring expertise in device fabrication, while Mohney's students may help them to look at samples with the TEM or help them better understand the thermodynamics of the materials system within which they are working. The Mohney group has also collaborated extensively with the Joan Redwing group on research into contacts to silicon nanowires, and with many other groups within MSC and on campus.

Anna Domask has a Master of Science and is currently pursuing her Ph.D. in materials science. After earning her undergraduate degree at Cornell University, she worked as a consultant for the DOE Hydrogen, Fuel Cells, and Infrastructure Technologies Program. She is the instructor for a general education Penn State World Campus online course that teaches materials science in the context of history and world events. The course is open to anyone. She can be contacted at acd184@psu.edu. Suzanne Mohney's website is http://www.esm.psu.edu/mohney/.



Materials Day 2013 Materials for Emerging Technologies

In a change from the traditional early spring meeting, this year's Materials Day was held in October. The weather was perfect, the autumn leaves were at their peak, and the University Park campus was idyllic. On Tuesday evening, graduate students and faculty mingled with visitors from industry at a reception sponsored by Corning, Inc. in the Nittany Lion Inn ballroom. Corning's chief technology officer, David Morse, gave a keynote address on the future of technical glass and Corning's commitment to research. Earlier in the day, Penn State faculty and staff presented seven ninety-minute tutorials on topics ranging from advances in nanofabrication to 3D printing for additive manufacturing. Tours of Penn State's state-of-the-art Millennium Science Complex were offered in the morning. Day two was busy with five plenary talks, followed by lunch and an interactive poster session with faculty and students presenting 120 posters. For the complete summary of talks, visit our Materials Day pages at mri.psu.edu under News/Events.



Maryam Sarkarat, a post-doc in mechanical engineering, discusses her poster at Materials Day 2013.

Two Laboratories One Integrated Solution...

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TEM image of a vertical TFET Credit: Datta group, Penn State

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> Bill Drawl, Nanofab Research and Development Engineer



New, High-Impact Next-Generation Transistor

Prof. Suman Datta's group is using the capabilities of the Nanofab and MCL to develop new kinds of transistors that could be key components in a future generation of logic and memory devices. These tunnel field effect transistors (TFET) are designed to replace current CMOS transistors using materials such as gallium arsenide antimonide / indium gallium arsenide as source, channel, and drain, or a strained germanium layer as the active component in the transistor. E-beam lithography and atomic layer deposition are among the tools the group uses to build prototypes in the Nanofab, which can then be characterized one floor below using the extensive suite of tools and techniques in the MCL. Through each step of the process, highly trained technical staff in both labs help the researchers obtain and interpret their data.



Reciprocal space map shows strain in germanium lave of transistor Credit: Datta group, Penn State

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