INquiry

Science and Technology at the Ames Laboratory

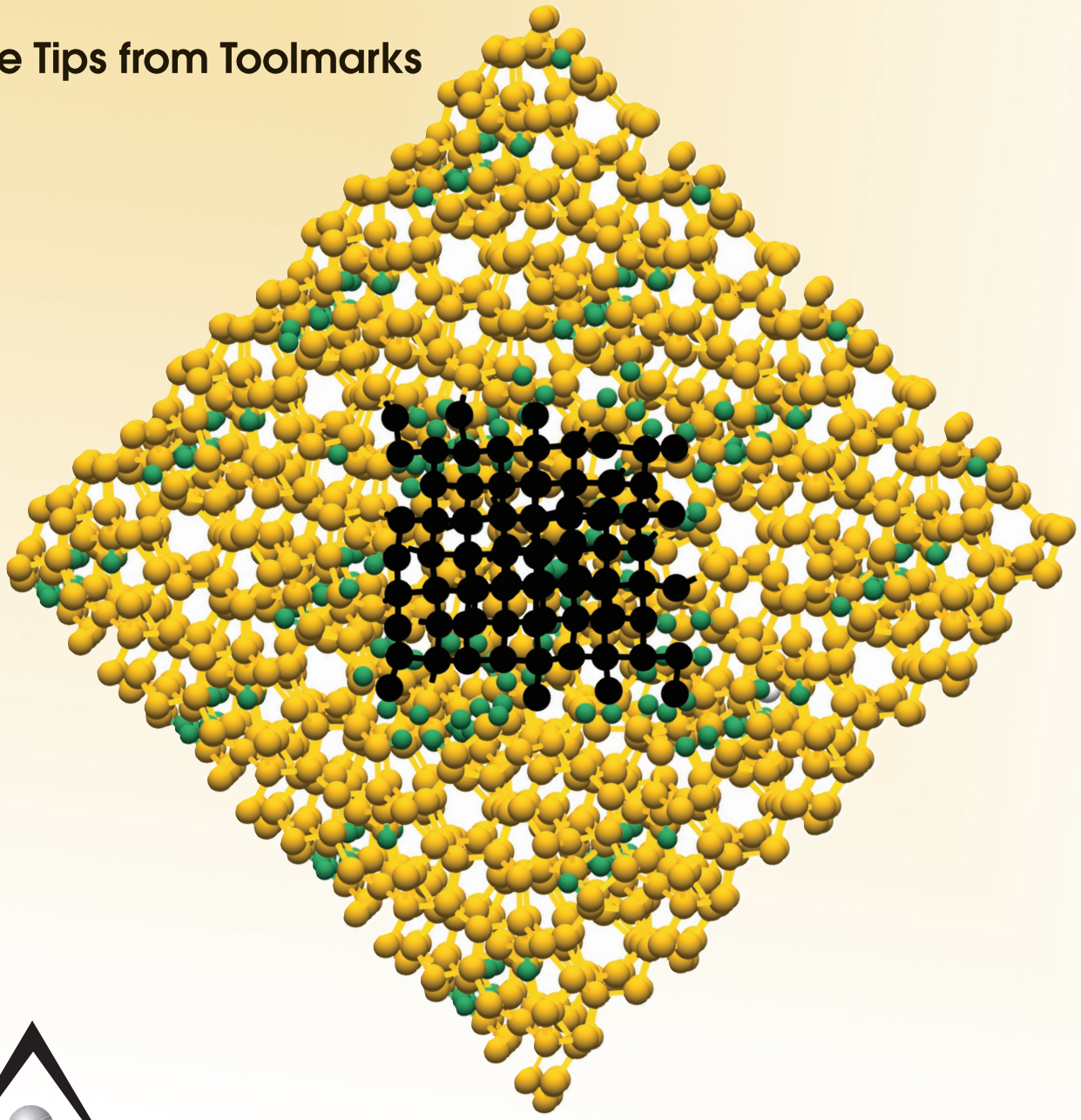
2003

New-generation Catalysts

R&D 100 Winner

Guiding Neuron Growth

Crime Tips from Toolmarks



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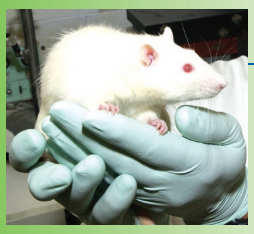

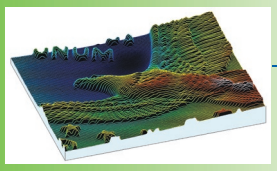

(front cover) This molecular dynamics simulation shows a new mixed-phase solar cell material consisting of clusters of nanocrystalline silicon embedded in an amorphous matrix. The material is proving more stable in sunlight than traditional amorphous materials. (see story page 8)

(back cover) A well-used lab notebook and cardboard coffee cups converted to pencil holders — sure signs that a busy graduate student "lives" here.

from the *Director*

We are indeed pleased to begin this issue of *Inquiry* by congratulating Marc Porter, Ames Laboratory associate, and his colleague Robert Lipert for winning an R&D 100 Award in 2003. Marc and Bob have been working with a company to develop the Ramanprobes System for detecting and labeling antibodies, proteins that serve as the body's natural defense system against infectious agents.

Beyond this R&D 100 recognition, Ames Laboratory scientists continued to perform innovative basic and applied research in a variety of key scientific areas over the past year. Our cover story features research that may finally answer a perplexing question that has plagued the research community for more than 20 years: Why do solar cells degrade in sunlight? Research by physicist Rana Biswas and his co-workers is shedding new light on the atomic origins of light-induced degradation. It is hoped that this work will lead to improved efficiency and reliability in solar cells.

While Biswas deals with solar cells, Surya Mallapragada is concentrating her efforts on human cells by spearheading research to re-grow nerve cells. Her innovative research uses an ultrathin biodegradable polymer to form a bridge between severed nerves that provides a path for neurons to reconnect. The polymer is already showing great promise in tests on the sciatic nerves in test animals.

In other cutting-edge research, Victor Lin is involved in innovative work on a new generation of highly selective and efficient catalysts that can be tailored to specific classes of chemical reactions. These catalysts may be used in the synthesis of new polymers and fuels.

Ames Laboratory's Mark Gordon is leading a group that is expanding a computational chemistry code that provides extensive and detailed information on how things work on the molecular scale. The software, called GAMESS — General Atomic and Molecular Electronic Structure System — may serve as the foundation for the design of new fuels and optical materials and the development of coatings that are resistant to extreme environments.

In the area of forensics, Laboratory researchers Stan Bajic and David Baldwin are spearheading a project that supports "toolmark" identification as a method for helping connect tools found on suspects to the crimes. The project includes an image database and software tool that ultimately may help the courts put more criminals behind bars.

These are just a few of the fascinating research efforts underway at Ames Laboratory that you can read about in this issue of *Inquiry*. I think you'll agree our scientists are doing some very exciting things in their efforts to find solutions to our nation's energy problems.

Tom Barton

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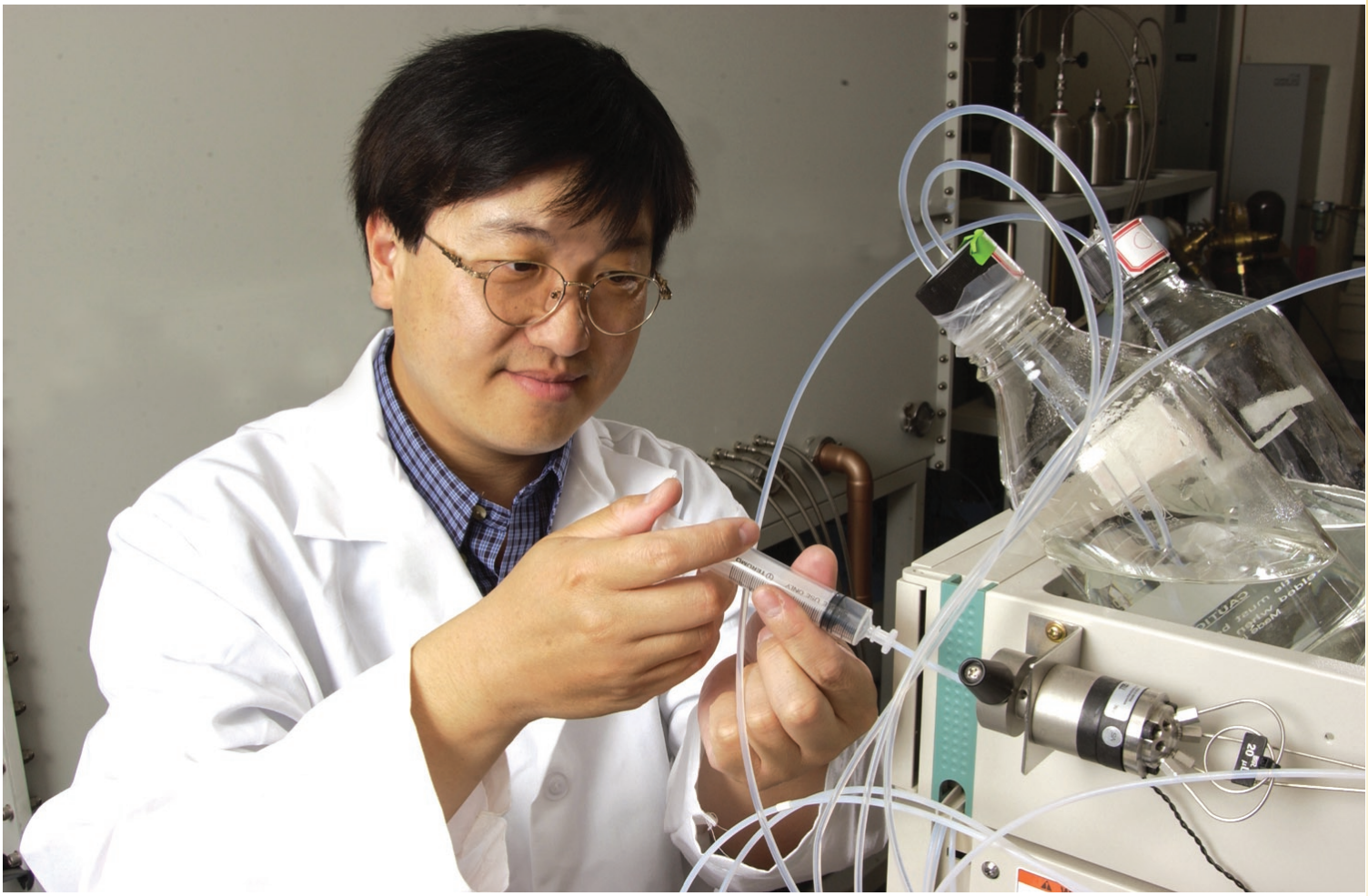
Hanging Picassos

by Saren Johnston

"Gatekeeping" strategy promises more active catalysts



Victor Lin injects a sample of products synthesized by a gatekeeper-functionalized mesoporous nanocatalyst into a high-performance liquid chromatography apparatus. The yield and purity of the desired product are being analyzed by the HPLC.

Victor Lin likes to explain his research on improving the efficiency and selectivity of catalysts from an artistic point of view. "Suppose you're walking through a museum and you pass a showroom in which the walls are decorated with Picassos," he says. "You can enter the room if you want — nothing is blocking your way. But if you don't happen to like Picasso, you might see this room and think to yourself, 'Well, I can go in there, but I prefer not to,' and you pass it by. That's exactly the idea that we use in our gatekeeping strategy to prevent various reactants from accessing specific catalysts," says Lin, an Ames Laboratory chemist and an Iowa State University assistant professor of chemistry.

Material matters

Catalysts are substances that speed up the rates of chemical reactions without getting used up in those reactions themselves. And mesoporous inorganic materials are the current craze in scientists' efforts to enhance the catalytic process due to their heterogeneous nature. The possibility of incorporating various catalytic functional groups into the characteristically large and uniformly arranged porous channels of these materials, allowing control on a nanometer scale, makes them ideal candidates for use as catalysts that can be easily separated from the products and recycled.

"These mesoporous materials are called nanoporous catalysts because their pore size is typically within one hundred nanometers," explains Lin. The pore diameters are chosen to control the access of molecules to the catalytic reaction sites located inside the porous cavities of the material. Only the molecules of certain sizes and chemical properties are selected and guided to the reaction centers where they are efficiently transformed to the desired products. "That creates some very interesting catalytic effects," says Lin.

Although mesoporous materials with their large surface areas are well suited to the task of enhancing catalytic activity, problems

More than just pretty piles of powder. The white powder on the upper left is mesoporous silica nanosphere (MSN) material. The light blue and pale yellow powders are the MSN functionalized with copper and palladium catalysts, respectively. These mesoporous materials can catalyze the syntheses of various conductive polymers and structurally align the molecular wire products. The gold and black powders are the copper- and palladium-MSN catalysts with their pores filled with two different conductive polymer products.

can arise in terms of selectivity. "Presumably reactants can enter the material from all different angles, so this kind of catalyst will not provide the kind of selectivity you would like to have," says Lin. "Let's say you have two reactants, A and B, in your starting material and both will react with your catalyst. But you only want the product from reactant A, so you have to find a way to get rid of reactant B."

According to Lin, it often requires costly and time-consuming separation techniques to produce a pure starting material containing only reactant A.

Offering a real-world example, Lin notes that currently there is a lot of interest in generating biodegradable polymers. "Probably the most commonly used polymer these days is all petroleum-based," he says. "Some day we'll use up petroleum — that's one thing. The other thing is that these polymers are not biodegradable. So, if you could actually create biodegradable polymers with chemical and mechanical properties that mimic those of petroleum-based polymers, then you could presumably use them to replace petroleum-based polymers. So there is tremendous interest in this area."

The problem is that petroleum chemistry has been around for two centuries so all the infrastructures are well established. "You can get some cheap starting materials — something really pure and economical to play with, whereas in the bio-related world, your starting materials are typically a mixture," Lin says. "You have all kinds of different things, so separating, or fishing out, the right kind of starting materials is usually labor-intensive."

Nature's natural roadblock

Separating reactants is often an enormous job thanks to a little quirk of Mother Nature called chirality in which a three-dimensional form, such as a person's hand, is different from its mirror image. Any object that cannot be superimposed on its reflection is said to be chiral, and this is the situation that exists with certain molecules.

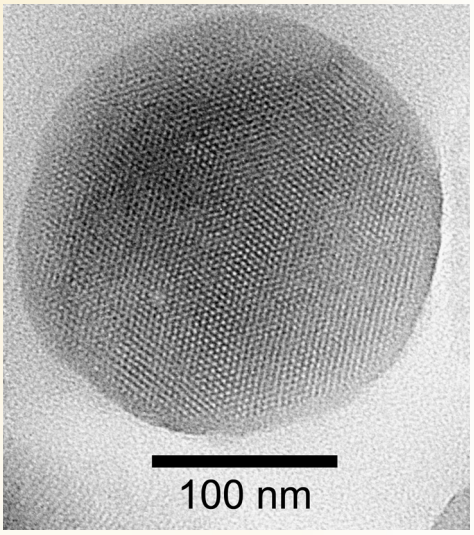
"Chiral molecules look identical, but you cannot superimpose them," says Lin. "They have the same number of atoms and the same type of composition, but they have totally different properties. People have been doing chiral separations for years, and they've been very successful at it, but there is no direct connection between that separation world and the catalysis world," he adds. "You don't have such an integrated package."

Lin explains that scientists working in the area of catalysis must rely on separation science experts to purify the starting materials for specific reactions. "Then they hand them down to the catalysis people," he says. "But this is not all that feasible anymore because the separation costs have become extremely high."

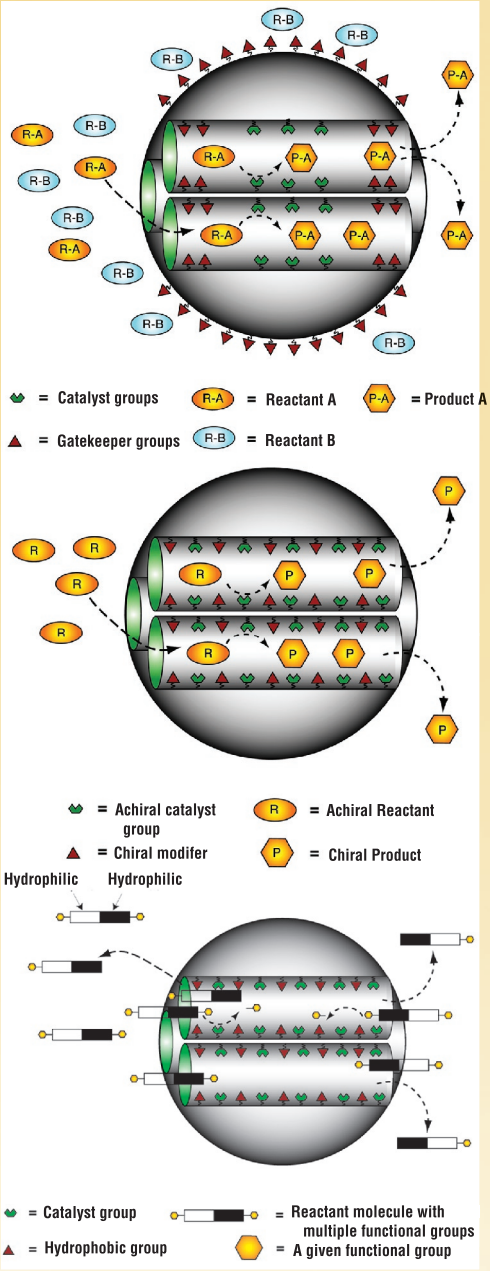
Incorporating the separation work into the catalyst seemed a likely way to bypass the time and expense associated with chiral separation. So Lin and his co-workers began using MCM-41 type of mesoporous silica materials, also referred to as Mobil Chemical Material 41 silica, to prepare nanocatalysts that would include this innovative feature. Making use of the porous channels comprising the MCM silica, they created a honeycomb-type structure and attached catalytic functional groups to individual sites on the pore walls and at the entrances to the individual channels.

"The catalytic groups, themselves, have absolutely no selectivity whatsoever," says Lin. "They're just simple and often commercially available catalysts. That's why they're cheap and easily synthesized. But we still want the selectivity," he reminds us. "So what do we do?"

Resolving the selectivity problem involved installing chiral selectors, or "gatekeepers," as Lin likes to call them, with the MCM mesoporous catalysts. These gatekeepers are synthetic compounds or natural products that have a specific chirality, so they deter unwanted reactants from reaching the catalyst. "If only one reactant is allowed to react with the catalyst, you could actually accomplish stereochemical control without employing very sophisticated and often expensive asymmetric catalysts," says Lin. "And you can play a lot of games with this kind of strategy."



This transmission electron microscope image shows a cross-section of a mesoporous silica nanosphere. The pores are represented by the hexagonally packed dots.



Lin's three methods for anchoring catalysts and chiral (or other structural) promoters to the pore surfaces of MSN catalysts are:

Top: Gatekeeper groups allow only reactant A to enter the mesopores to yield the desired product A.

Middle: Chiral promoting groups are placed next to catalytic functional groups inside the "decorated" mesopores. The proximity may cause the catalysts to preferentially generate a product with the desired chirality.

Bottom: In a process called "domain selective catalysis," the interior pore surfaces of the mesoporous catalyst are decorated with hydrophobic gatekeepers so that only those functional groups on the hydrophobic part of the molecule enter the pore and react with the catalysts, whereas the same functional groups on the hydrophilic side of the molecule cannot be converted to products.

Deck the "walls"

Exploring various approaches for designing and fine-tuning the degree of functionalization of these single-site mesoporous catalysts involves what Lin refers to as "decorating the walls." In a sense, he's hanging his own Picassos, anchoring catalysts to well-defined sites at the entrance to and on the channel walls of the mesoporous material, creating a "museum room" adorned in a way that is inviting to only a specific reactant. Although other reactants could enter, they prefer not to and pass on by, much like the museum visitors in Lin's analogy who chose not to enter the room decorated with Picassos.

Lin has devised three unique schemes for anchoring the groups of catalysts and gatekeepers, or chiral promoters, within the mesoporous, honeycomb-type structure. "The first idea was to decorate the outside of the channels with a certain chiral promoting group that allows only one reactant, let's say reactant A, to enter the catalyst, so only product A is generated," he says.

The second method involves decorating the inside of the mesoporous channels by placing the chiral promoting groups right next to the catalytic functional groups. Although the catalysts don't have any chiral promoting abilities themselves, the proximity to the chiral groups may cause them to preferentially generate some sort of chiral product.

Huge molecules known as macromolecules play a key role in Lin's third scheme for installing gatekeepers. Similar types of functional groups, such as acid groups, may be attached to each end, or pole, of a macromolecule. "Those chemists who want to functionalize an acid group on one side of the macromolecule must somehow protect the other acid group on the opposite side," says Lin. "So protection and deprotection processes will be needed."

Offering a way to circumvent those processes, Lin says, "In the case of a molecule that has one pole hydrophobic and the other pole hydrophilic, we could play a trick and decorate the interior pore surfaces of the catalyst with hydrophobic gatekeepers so that only the hydrophobic pole of the molecule would enter the cavity of the catalyst. The hydrophilic pole would stay outside of the catalyst with the water, and the hydrophobic pole would stay inside. In that way, we wouldn't need any protection processes," he adds, noting that this type of selectivity would greatly simplify the synthesis of many complex, biologically active molecules.

Catalyst collaboration

Lin says the three schemes for designing and tuning the highly selective mesoporous catalysts will undergo extensive scrutiny. He and Marek Pruski, Ames Laboratory physicist and co-principal investigator on the catalysis project, have already obtained several key preliminary results that demonstrate the feasibility of these new catalytic principles. Detailed characterization of these mesoporous catalysts has been provided by solid state nuclear magnetic resonance, or NMR, a spectroscopic technique that Pruski's group uses and develops. NMR offers unique information about the structure, location and dynamic behavior of molecules on mesoporous surfaces, which helps to understand how the catalysts work and drives further catalyst design.

Theoretical/computational modeling by Ames Lab researchers and co-principal investigators Mark Gordon and James Evans will provide state-of-the-art characterization capabilities for analyzing and predicting structures, molecular dynamics and reactivity in these systems. In addition, Lab researchers and co-principal investigators Robert Angelici, Andreja Bakac, James Espenson, and Edward Yeung will perform other catalytic studies, including kinetic, surface tethering, atom transfer, electron transfer and photochemistry, on the reactions that are catalyzed by the new nanocatalysts.

Controlling the structure and reactivity of the MCM mesoporous support material and how it interacts with the catalytic and chiral sites holds great promise for the design of a new generation of highly efficient and selective catalysts. In addition, the research efforts of Lin and his co-workers will expand the fundamental knowledge about catalysis in regard to selectivity, reactivity and kinetics. "We envision that this research will lay the foundations for the future development of a wide range of novel catalytic systems," says Lin. ◆

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INtouch

Ramanprobes Wins 2003 R&D 100 Award

"It's the assay system du jour," said Marc Porter. The Ames Laboratory associate and Iowa State University chemistry professor was speaking lightheartedly about Ramanprobes, the new-generation immunoassay system that he and Robert Lipert, a scientist at ISU's Institute for Physical Research and Technology, developed in association with Christian Schoen, president of Concurrent Analytical in Kailua, Hawaii. But the fact is, Ramanprobes is among the elite of today's new technologies, having been selected for a prestigious 2003 R&D 100 Award.

The R&D 100 Awards, sponsored by *R&D Magazine,* honor the top 100 products of technological significance marketed or licensed during the previous calendar year.

Ramanprobes is a highly sensitive labeling and optical detection system that can read multiple biomarkers, such as antibodies, concurrently at a single biochip address. Coupled with the selectivity of antibody binding, Ramanprobes allows quick detection and identification, and so has great potential for use within the medical arena. In emergency applications, it can expedite treatment for such infectious diseases as HIV, hepatitis C, smallpox and botulism. Another effort is centered on early cancer detection. Ramanprobes can also be used in military applications to detect weapons of mass destruction — all potentially close to single-molecule detection.

Crucial to the success of Ramanprobes is a new line of extrinsic Raman labels developed by Porter and Lipert with significant contributions from students in Porter's research group. Work on the optical detection nanotechnology began about five years ago, according to Porter. "In addition to Bob and myself, there have been six graduate students and a postdoc working on the project," he said, noting the team has at one time or another included the following individuals: Jing Ni, now at BioSpect in South San Francisco; Brent Dawson, now at the University of North Carolina-Greensboro; postdoctoral fellow Desiree Grubisha; and graduate students Hye-Yong Park, Jeremy Driskell, Betsy Jean Yakes and Jill Uhlenkamp. "That's the gang, so to speak, the people who make it all happen," said Porter.

While Porter and Lipert headed up the work on the extrinsic Raman labels and the biochip development for the Ramanprobes technology, Schoen led the effort to build the compact, lightweight fiber-optic Raman system, the NanoRaman I Instrument. Together, the new labels and the Raman instrument offer a unique optical detection technology with significant advantages over state-of-the-art fluorescent systems, including greater sensitivity, enhanced concurrent analysis and instrument simplification.

"The long-range goal is to build a chip that has several different addresses, or antibodies, on it," Porter explained. "The idea, in the end, is to be able to screen for multiple biomarkers. In early disease detection or diagnosis, the sooner you can detect the occurrence of a disease state, the greater the likelihood of a successful treatment outcome."

R&D 100 winners for the Ramanprobes ™ System (left to right): Marc Porter, Iowa State University; Christian Schoen, Concurrent Analytical, Inc.; and Robert Lipert, Iowa State University.

Describing how the biochip is constructed and the placement of the extrinsic Raman labels on the chip, Lipert said, "The chips are just little gold-coated pieces of glass. On top of the gold substrate, we place antibodies for whatever it is we want to detect. The purpose of those antibodies is to selectively capture the antigens from the sample." He explained that the gold-bound antibodies capture the antigens as part of a detection scheme known as a sandwich assay. The next step exposes the captured antigens to more antibodies that also bind to the captured antigens.

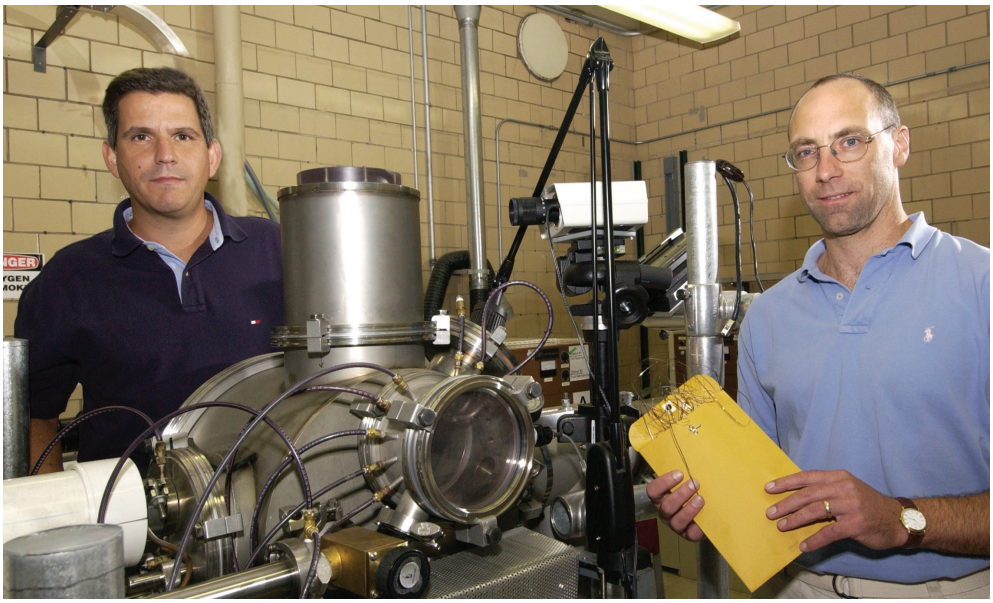
"The issue is to have some way of signaling that the captured antigens are there, and just binding another antibody isn't enough for the sensitivity needed for many emerging applications," Lipert continued. "We need to label that antibody with something we can detect at very low levels." The labeling process involves placing the antibodies on gold nanoparticles, 30-80 nanometers in size, which are also derivatized with Raman labels. Gold nanoparticles are used because when a laser beam is shined on them, they greatly enhance the spectroscopic signal from the label molecules.

"In the past, a lot of these kinds of assays were done with fluorescence labeling," said Lipert. "Most of these fluorescence labels give very broad spectral features, so there are a limited number of labels that you can distinguish concurrently. The advantage of the Raman labels is that their spectral features are much narrower, and you can think of them more as a fingerprint. So you could conceive of an assay where you are able to detect many different labels for many different antigens simultaneously."

Porter elaborated, "You'd focus the laser light on one spot, collect the light that's being scattered by the sample, analyze it with the monochromator and pick out the different components. So far, we've detected three different antigens simultaneously, but we think we can get up to 30 at one time. We have some ideas on how to do it, but now we're focused on improving sensitivity and reproducibility — learning how to do the measurements on just a couple of them really well first before we try to branch out." ◆

Unlocking the Mystery of *Amorphous Materials*

by Kerry Gibson



Dan Sordelet, left, and Matt Kramer stand next to the melt spinner that provides the metallic glass samples they're studying. By devitrifying melt-spun materials, they hope to determine how these amorphous materials form in the first place.

Here's a riddle for you. When does a metal not act like a metal?

Give up? When it's a glass.

Though that question would stump most of us — even when we have the answer — it's a no-brainer for Ames Laboratory researchers Dan Sordelet and Matt Kramer. The real riddle for them is why metals take on various glass-like structures and properties depending on how the materials were processed.

By definition, glass — including the common window variety — is formed when a material is synthesized in such a way that a regular crystalline structure isn't formed. This random, or amorphous, arrangement of atoms gives metallic "glasses" a number of unique physical and sometimes electrical and magnetic properties. Compared to their crystalline counterparts, metallic glasses are more rigid, yet can be formed into complex shapes well below their melting temperatures.

Normally, metals have a very regular, or periodic, structure in which the atoms align. This ordered arrangement contains damage mechanisms that allow crystalline metals to be permanently bent or dented. The glass form of a metal lacks that regular pattern to its atomic structure, making it both hard and elastic, giving it the ability to snap back into its original shape instead of deforming — as long as it's not bent too far. The stress it takes to deform the glass this incremental amount is much higher compared to many typical metal alloys. These fascinating materials are difficult to study, however, because of the ways and speeds with which they form.

"We're studying materials that have been melt-spun — basically a stream of molten metal is dropped onto a spinning copper wheel and solidifies in a ribbon before the atoms can line up," Sordelet says. "Another way to create a metallic glass is to use high-energy mechanical deformation, e.g. mechanical milling to basically destroy the crystal structure to such an extent that it becomes amorphous.

"We've also worked with Pal Molian, an Iowa State University mechanical engineering professor, to use a laser to vaporize materials into highly energetic atoms and have them condense randomly in a thin coating," Sordelet adds. "But with all of these contrasting synthesis methods, it's difficult or impossible to find out what's taking place at the atomic level as the amorphous structure forms."

Working backwards

To get an idea of how the atoms are arranged in a particular amorphous structure, the two researchers work backwards, so to speak, through a process called devitrification. Basically, it involves gradually heating the metallic glass until it devitrifies — loses its amorphous properties — and the atoms realign in the metal's regular crystalline pattern.

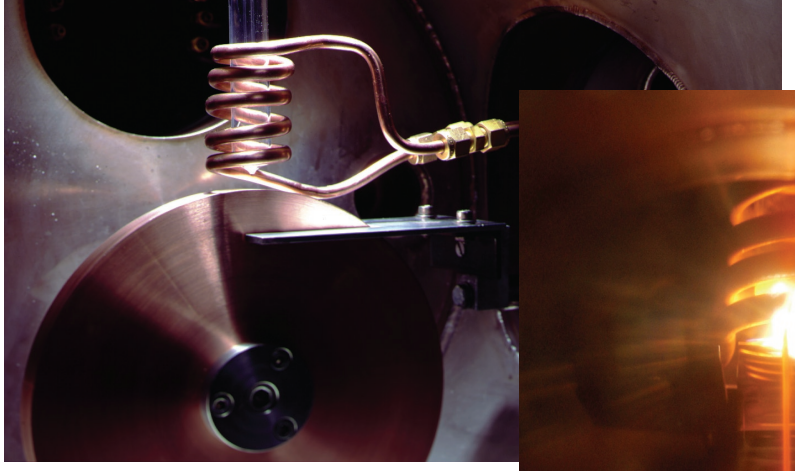
Early results show that as they are gradually heated, certain metallic glasses have an intermediate, metastable quasicrystalline phase before returning to their normal periodic structures. But whether a metastable structure forms, and what type of structure occurs, appears to depend on how the metallic glass was originally created. Sordelet and Kramer speculate that how the metallic glass is made is closely linked to its original amorphous structure.

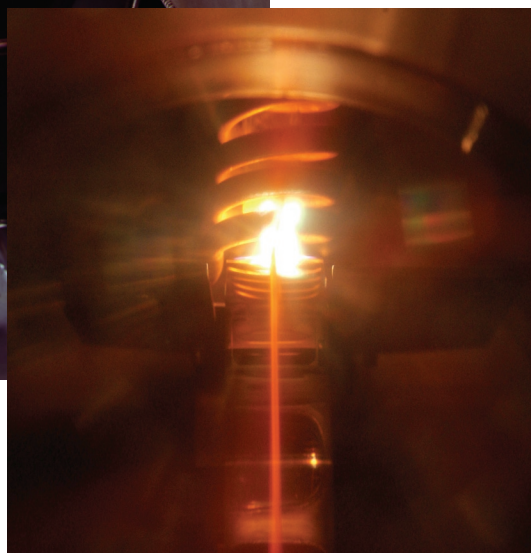
"Material that was melt-spun forms these intermediate quasicrystalline phases clearly during devitrification," Sordelet says, "while mechanically milled material does not transform into these metastable transition states. We're trying to determine why these differences exist."

Think golf green

Kramer draws an analogy to a golf putting green to better illustrate the point.

"You've got balls at various points on the green," he says, "and while they all ultimately end up in the cup, they take very different paths getting there. Some go fairly straight in while others follow dips and breaks traveling to the hole. The devitrification pathway is going be different depending on the material's initial state — where the balls start from on the green.





At the heart of the melt spinner is a copper wheel. An induction coil melts the material being studied, and a stream of liquid metal drops onto the spinning copper wheel. Because copper dissipates heat extremely well, the liquid metal solidifies so quickly that it doesn't have a chance to form in its normal, periodic crystal structure and forms as an amorphous metallic glass.

"The balls' starting positions on the green are linked to how they were made," Kramer continues.

"For example, the ball representing the melt-spun metallic glass might have several valleys, i.e. metastable structures it must roll down into and up out of before finally reaching the hole. If not hit firmly enough, the ball could get stuck in one of these valleys, which is analogous to the amorphous melt-spun ribbon transforming into a metastable quasicrystalline structure."

Because the quasicrystalline phase occurs when a metallic glass formed from a liquid is heated, but not in a metallic glass created by solid-state mechanical deformation, the two researchers speculate that even though the liquid-formed glass appears to be amorphous, its structure isn't truly random. Some unidentified alignment of atoms is carried over from the liquid that is similar to the symmetry of the initial metastable phase that forms.

In the specific case where metastable quasicrystals form, many researchers have proposed that an icosahedral short-range order exists in the liquid prior to quenching it into a glass. This local order is retained to some degree in the glass, and the similarity of its structure with the long-range structure of the quasicrystals is energetically favorable to form the intermediate quasicrystal structure. Upon further heating, this intermediate structure ultimately transforms into the stable structure for the particular metallic alloy.

"From a fundamental viewpoint, we want to try to make the linkage between the structure that's in a liquid and the resulting amorphous structures that we see," Kramer says, "and identify the relationship of the short-range order in the glassy alloy and the role it plays in phase selection as the materials devitrify."

Keeping it simple

To help simplify the task, Kramer and Sordelet have focused on binary alloys, such as zirconium-palladium, because of the limited number of ways the materials can bond together. Minimizing the possible configurations also helps Ames Laboratory physicist James Morris, who is working on developing theoretical models, to explain what's happening.

The interdisciplinary team is also relying on some powerful, high-tech tools to analyze the materials, such as the Advanced Photon Source synchrotron radiation source at Argonne National Laboratory. Using a novel furnace Kramer helped design and build for the Midwest Universities Collaborative Access Team at APS, the team gradually heats samples of $Zr_{70}Pd_{30}$ while using the high-energy beam line radiation to produce X-ray diffraction images of the material's atomic structure.

"High-energy synchrotron radiation is able to probe the entire sample in a time span that's rapid relative to the heating rate of the sample," Kramer says. "That's critical to understand the average behavior of the bulk and not just the few microns near the surface."

To take some different "snapshots" of the materials, Sordelet and Kramer are collaborating with researchers from the Centre National de la Recherche Scientifique at the Ecole des Mines in Nancy, France, to utilize accelerator facilities in Oxford, England, and Grenoble, France, where neutrons are used to bombard the samples instead of photons. According to Kramer, this will complement the X-ray technique and provide information on the static conditions.

To augment their work with metallic glasses, the two researchers are making use of a relatively new and unique binary quasicrystalline alloy: cadmium-ytterbium. This system shows even more promise to help unlock the mystery of icosahedral short-range order in liquids because it is quasicrystalline and melts directly from the solid to the liquid without a change in composition, a process known as congruent melting. This approach should take even more variables out of the equation since it's known that the solidifying phase contains icosahedral order.

"We're fortunate to be able to work with Tom Lograsso, an Ames Laboratory senior metallurgist," Sordelet says, "since he's developed methods for working with this alloy to produce large-scale, single-grain crystals not available anywhere else."

While the researchers admit they aren't precisely sure where their work will lead in gaining new fundamental insight into the infinite range of amorphous structures of metallic glasses, there could be some practical applications that come out of it. Kramer points out that one of the keys to forming nanoscale materials is to control devitrification.

"When we form something that's amorphous and then heat it up, what crystallizes are typically nanocrystalline structures 5 nanometers to 25 nanometers in size," Sordelet says, "and that has importance in the development of magnetic and high-strength materials." ◆

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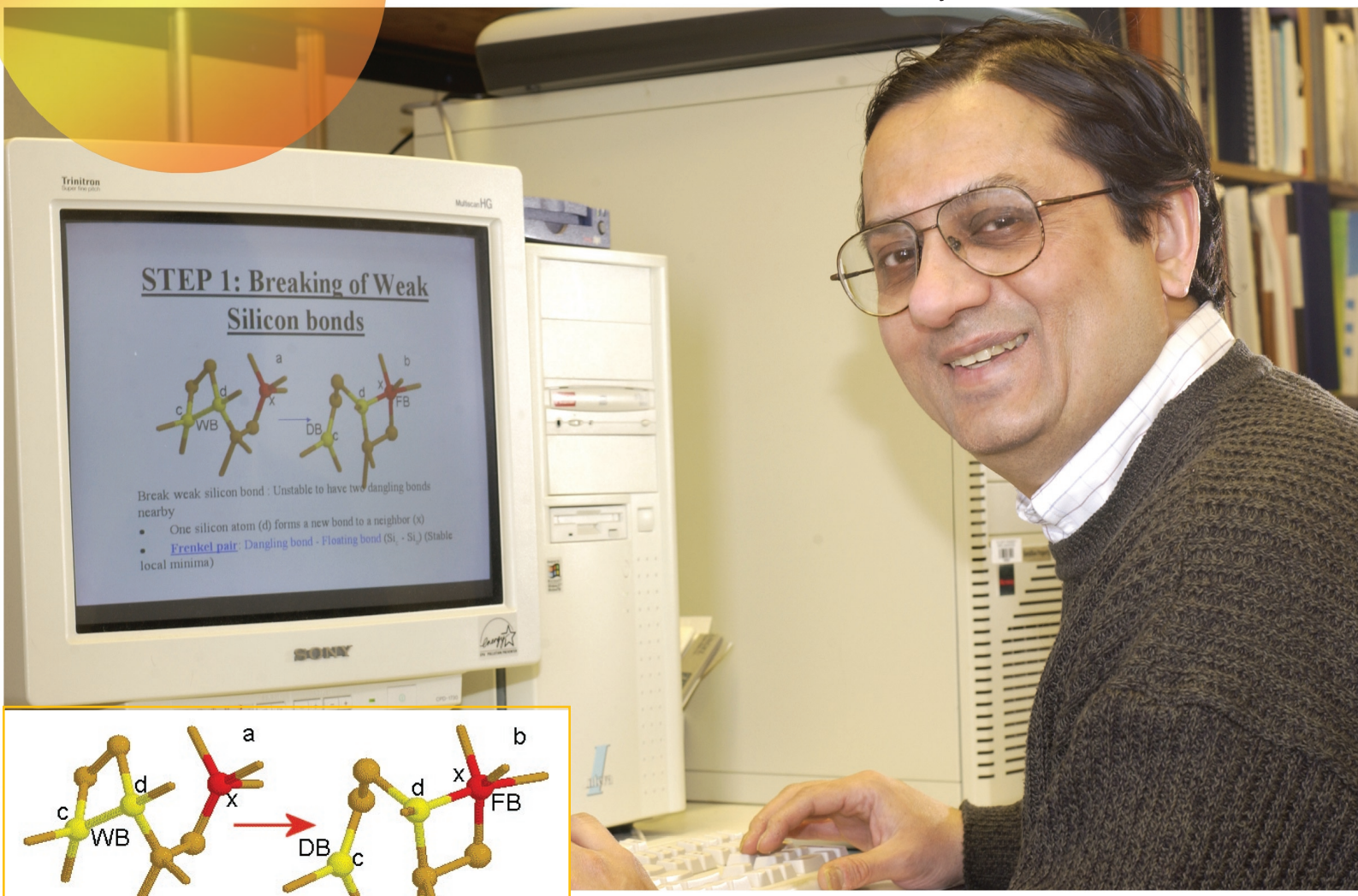
Sunproofing Solar Cells

by Saren Johnston



Rana Biswas may have found the answer to why solar cells degrade in sunlight and has developed computer molecular dynamics simulations to describe the three-step process. Pictured on the computer screen and the inset image is the first step in his network rebonding process — the breaking of weak silicon bonds in the hydrogenated amorphous silicon solar cell material. In the figure on the left of the insert, the weak bond (WB) between atoms c-d has broken, creating, in the figure on the right, a dangling bond (DB) on c and a new bond, d-x, which results in a floating bond (FB) at x.

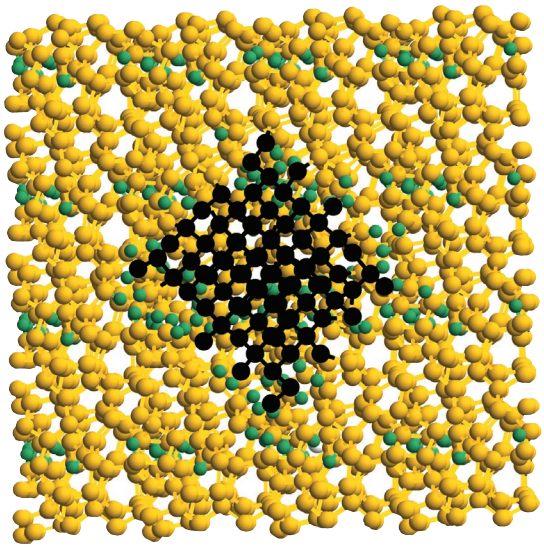
When it comes to sunlight, any dermatologist will tell you a little goes a long way. But who would have thought the same warning would apply to solar cells — the collection vessels for energy from the sun.

Solar cells degrade in sunlight — a mysterious fact that has plagued the research community for more than 20 years. Discovering how that degradation process takes place is essential to the advancement of solar cell research and the ability to produce lower-cost electricity from sunlight.

Sun damage

"The basic problem is that when you put solar cells in sunlight, the efficiency starts to decrease by as much as 15 percent to 20 percent over a period of several days," says Rana Biwas, a physicist at Ames Laboratory and Iowa State University's Microelectronics Research Center. "Obviously, that's not good." He notes that it's possible to reverse the effect by heating the solar cell material in an oven to 170-200 degrees Centigrade (338 F-392 F), but adds that's not possible to do in practice.

Solar cells made from hydrogenated amorphous silicon, a noncrystalline form of silicon, absorb light far more effectively than traditional crystalline silicon solar cells. "In-



A new material consisting of clusters of nanocrystalline silicon embedded in an amorphous matrix holds promise for an improved generation of solar cells that are more stable in sunlight than today's technology.

stead of a thick, 20-micron crystalline silicon film, you can just deal with a very thin, half-micron amorphous silicon film," says Biswas. "These cells are more cost-effective as they involve much less material and processing time — driving forces for industry. However, although amorphous silicon absorbs light very efficiently, it suffers from this degradation effect — that's the bad news."

Biswas and his co-workers, Ames Lab visiting scientists Bicai Pan and Yiying Ye, have been studying the troublesome degradation effect, also known as the Staebler-Wronski effect, for the past few years. The research includes investigations into the atomic origins of the S-W effect and the subsequent exploration of possible new solar cell materials through computer molecular dynamics simulations. The work is part of both the Beyond the Horizons project and the National Amorphous Silicon Team effort within the Thin-Film Partnership Program, both cost-shared development programs of the Department of Energy's National Renewable Energy Laboratory.

A "bonding" experience

Biswas explains that exposure to light can cause changes in hydrogenated amorphous silicon, resulting in defects known as metastable dangling bonds — bonds that can go away only when heated to a high temperature. Dangling bonds are missing a neighbor to which they can bond. To remedy the situation, they will "capture" electrons, reducing the electricity that light can produce and decreasing solar cell efficiencies. "The question," Biswas says, "is how does light create the dangling bonds?"

With the development of their three-step atomistic rebonding model, Biswas, Pan and Ye are well on the way to resolving many puzzling aspects of the problem. The model is based on rearrangements of silicon and hydrogen atoms in the hydrogenated amorphous silicon material.

In the first step of the three-step process, sunlight creates excited electrons and holes (vacant electron energy states) in the material. When the electrons recombine, they pair up with holes on the weak silicon bonds. The recombination energy causes the weak silicon bonds to break, creating silicon dangling bond-floating bond pairs. During the second step, the floating bonds break away from the dangling bonds and move freely throughout the material. This occurs when the extra floating bond from one silicon atom moves to a neighboring silicon atom. The third step reveals that the short-lived floating bonds disappear. Some recombine with the silicon dangling bonds, which results in no material defects. Others "hop" away from the dangling bonds and are annihilated when hydrogen atoms in the network move into the floating bond sites.

Biswas' three-step rebonding model shows that defect creation in hydrogenated amorphous silicon solar cells is initially driven by the breaking of weak silicon bonds followed by the rebonding of both silicon and hydrogen sites in the material. The research represents a significant achievement in understanding the atomic origins of the light-induced degradation effect in hydrogenated amorphous silicon and so provides a vantage point for eliminating this effect in the development of new solar cell materials — a task on which Biswas is now focusing his efforts.

A splendid blend

To improve the efficiency and reliability of solar cells, Biswas and Pan are investigating mixed-phase solar cell materials that consist of clusters of nanocrystalline silicon embedded in an amorphous matrix. "One of the most promising developments has been the success of hydrogen-diluted materials grown at the edge of crystallinity — the phase boundary between microcrystalline and amorphous film growth," says Biswas. "Our findings show that the crystallites make the mixed-phase materials quite stable, with the exception of the grain boundary region.

"There's a great deal of strain at the grain boundary because of the mismatch of materials, so we have a lot of excess hydrogen in the grain boundary," he explains. "The role of hydrogen is critical because weak silicon bonds, dangling bonds and floating bonds are all removed by hydrogen insertion."

The mixed-phase materials and solar cells made from them have a much greater stability to light-induced degradation than traditional amorphous materials. By developing molecular dynamics computer simulations, Biswas hopes to learn more about the mixed-phase materials at the atomic level and discover what aspect or aspects of the materials are responsible for the improved properties. His research efforts may even extend to manipulating the nanoscale structure of the material, allowing the design and creation of improved solar cell materials. ◆

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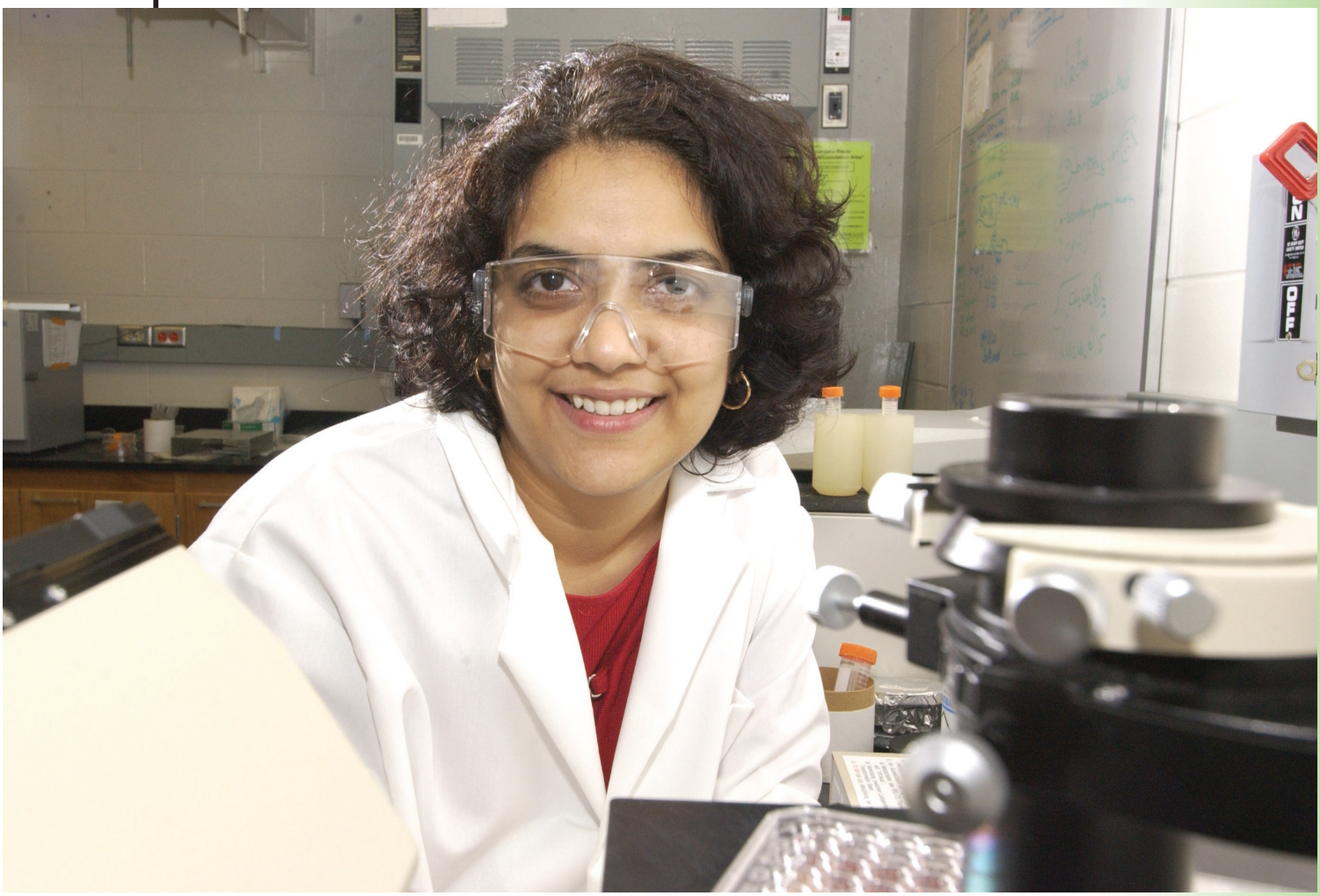
Groovy Plastic Helps Rebuild Nerves

by Kerry Gibson



Surya Mallapragada has developed methods to put nanoscale grooves on thin polymer films. The grooves help steer nerve cell growth to allow the "rewiring" of damaged nerves.

It takes a powerful microscope to actually see what Surya Mallapragada has developed, but its impact could be huge, especially for millions of people with various forms of paralysis. Micrographs showing tiny nerve cells growing along in an orderly fashion demonstrate how important this breakthrough could be in the ability to rewire broken nerve circuits in the human body.

Mallapragada's technique uses microscale channels cut in an ultrathin biodegradable polymer to regrow nerve cells. The method has already been proven to work for peripheral nerve regeneration in laboratory rats, and it may one day allow the paralyzed to walk and the blind to see.

Bridging the gap

Nerve cells are unlike most other biological tissue. When a nerve is severed, the part of the neuron "downstream" of the injury typically dies off. And neurons in the human body can be several feet long. Grafting, which works well for other tissue such as skin, isn't the best option because it's difficult to get the nerve cells to line up and reconnect. There's also a loss of nerve function where the donor tissue is removed.

"Nerve cells aren't able to easily bridge gaps of more than one centimeter," says Mallapragada, an Ames Laboratory associate in Environmental and Protection Sciences and Materials Chemistry and a chemical engineering professor at Iowa State University. "Peripheral nervous system, or PNS, axons — the part of the nerve cell which carries the impulses — normally have a connective tissue sheath of myelin to guide their growth, and without that guidance, they aren't able to grow productively. They tend to branch out and form in knots."

Since the nervous system carries electrical impulses, it helps to think of nerve cells in terms of electrical wiring.

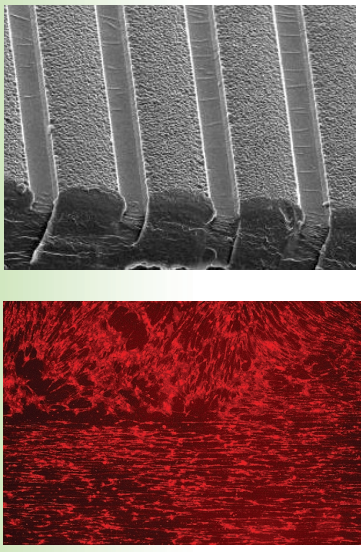
Bundles of nerves are like an electrical cable with multiple wires. When a nerve "cable" is cut and cells die, it would be as though the copper wire downstream of the damage disappeared, leaving only the empty plastic insulation tubes. In order for new copper wiring to push out across the gap and fill in the empty insulation tubes, you'd need a way to guide the wires into the empty insulation. And that's where Mallapragada's research comes in.

Grooves channel growth

By working on a cellular scale, she has developed a way to help guide neurons so they grow in the right direction. Starting with biodegradable polymer films only a few hundred microns thick (100 microns equals 0.004 inches — significantly less than the thickness of a human hair), Mallapragada and her colleagues have developed methods for making minute patterns on these incredibly thin materials.

"We've made grooves three microns to four microns deep to help channel nerve cell growth," Mallapragada says. "The grooves have a protein coating, and we've also 'seeded' them with Schwann cells to help promote this growth." Schwann cells naturally form the myelin sheath around the PNS cells. When guided by this sheath, nerves will grow at a rate of three millimeters to four millimeters per day.

The polymers, primarily poly(lactide-co-glycolide) and polyanhydrides, degrade when exposed to water, and



Micrographs of the polymer film show the grooved channels (top) and nerve cell growth in the polymer with grooves (lower half) and without (upper).

Mallapragada has worked to develop thin film polymers that bulk degrade in layers over a period of time ranging from a few days to almost a year. To put the microscale grooves in the polymers, she has used both laser etching and reactive ion etching, relying on the Ames Lab's Environmental and Protection Sciences Program and the Microanalytical Instrumentation Center's Carver and Keck Laboratories at ISU for the necessary equipment and expertise.

After promising in vitro tests, Mallapragada worked with biomedical scientist Srdija Jeftinija and other collaborators at ISU's College of Veterinary Medicine to conduct trials on rats. Small segments of the rats' sciatic nerves, which deliver nerve messages to the hind legs, were removed and the severed nerves "spliced" using a tube or "cuff" containing the polymer film.

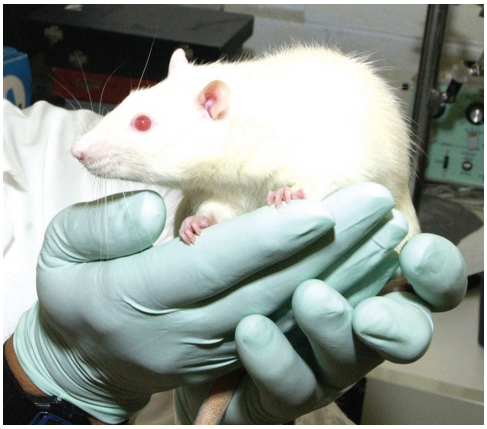
A suture at each end holds the cuff in place over the nerve ends. Though initially unable to move their legs, the rats started to regain use of their legs after three weeks and were able to function normally after six weeks.

Central nerve challenge

Although the technique has shown great promise with PNS cell growth, getting similar results with the central nervous system, which includes the brain, spinal cord and optic nerve, is another matter. CNS cells grow differently than peripheral nerves, presenting special problems. Oligodendrocytes, the connective tissue of the CNS, can actually inhibit nerve growth. Mallapragada has focused the next phase of her research on the optic nerve to try to better understand how CNS neurons work and grow.

"There are other factors at work, such as chemical and electrical cues," Mallapragada says. "Other researchers have had some success injecting adult (rat) stem cells into the site of the damaged optic nerve. Our hope is to eventually develop arrays of microelectrodes that will allow us to interface the optic nerve with a retinal chip … a bioartificial optic nerve, if you will."

The retinal chip, first developed at Johns Hopkins University, uses chip technology to replace the eye's rods and cones. The technology transfers



Rats similar to this one were used in the study on guiding neuron growth, in which a section of sciatic nerve was removed and the severed nerves spliced using the polymer film.

the digital images to the optic nerve via electrodes, but is limited by the inability to create electrodes that are small enough and numerous enough to create a resolution sufficient for the brain to decipher the input as it does with normal "sight."

"This research is a strong step forward in our basic understanding of nerve cell growth and how to engineer materials that help the body repair itself," says Ari Patrinos, Director of the Department of Energy's Office of Biological and Environmental Research. "We hope the groundwork laid by Ames Laboratory will soon pave the way for human subjects to benefit from this technology."

Mallapragada was honored for this and related polymer research in 2002 by being named one of the world's top 100 young innovators by *Technology Review*, a technology magazine published by the Massachusetts Institute of Technology. She is also associate director of the Microanalytical Instrumentation Center at Iowa State University. ◆

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Safe *and* SOUND

by Robert Mills

Norio Nakagawa is studying the use of eddy current inspection as one of the nondestructive evaluation technologies to be built into future nuclear reactors to continuously monitor their health.

Nuclear power plants are producing electricity at record rates, providing about one-fifth of our nation's electricity. Helping to keep them running safely are nondestructive evaluation technologies developed at Ames Laboratory. By providing the ability to peer inside critical pipes and structures without having to destroy them, NDE has become essential to the nuclear power industry.

Now, Norio Nakagawa, a physicist at the Ames Laboratory, and his collaborators are applying decades of NDE experience to future nuclear reactor designs. "We are giving NDE consideration while the system design is being developed. That's rather new in the nuclear business," Nakagawa says. The researchers are about two years into the three-year project, part of the U.S. Department of Energy's Nuclear Energy Research Initiative.

NERI's purpose is to address the long-term barriers to expanding the use of nuclear power to ensure that the United States can meet its future energy and environmental needs. The Ames Lab portion aims to develop concepts for on-line health monitoring of nuclear reactors to enhance the safety and economy of advanced nuclear power plants. In addition to Nakagawa, the research team includes R. Bruce Thompson and Feyzi Inanc of the Ames Laboratory as well as nuclear power industry representatives.

The on-line system will provide continuous monitoring so that deviations from normal operation can be detected immediately and problems can be addressed before they become serious. Moreover, on-line monitoring can be done remotely, greatly reducing exposure levels of maintenance workers.

Economics are also important, of course. "For nuclear power to be able to compete with other methods, it has to improve its operational costs," Nakagawa says. One way new reactor designs achieve this goal is by extending the refueling cycle to four years or more. This, however, makes today's "outage-based maintenance" approach problematic, where critical inspections are done when the plant is shut down for refueling, typically every 18 months. With the help of on-line health monitoring, designers of the next generation of nuclear reactors can reach the four-year goal to create plants that are safe and economically competitive.

Integrated inspections

The Ames Lab team is developing concepts that can be engineered into advanced nuclear reactor systems. "Our integrated inspection approach will help these systems achieve their goal of greatly enhanced safety and reliability," Nakagawa says. He adds that the team's concepts are generic enough to be used by designers of many types of nuclear power systems.

"The key is the on-line, integrated monitoring approach," Nakagawa says. The first step of the project has been to develop the overall concept. "Of course, there have been on-line sensors — temperature

gauges, and so on — but we are expanding the scope of the on-line sensor concept to the next level," Nakagawa says.

The second step of the project is to identify the most critical areas in need of on-line monitoring and then develop NDE concepts to address them. The Ames Laboratory researchers are also developing sensitivity estimates for each technology. "That will tell us how much sensor output to expect," Nakagawa says.

The first area is steam generator tubing. As the name indicates, a steam generator boils the secondary water into steam that goes to the turbine. Steam generators require a fair amount of tubing to maximize heat transfer efficiency from the core to the steam. "The tubing is very important in terms of safety inspection," Nakagawa says. One potential problem is magnetite deposits, iron oxide that builds up where the coolant in a steam tube evaporates. The magnetite buildup reduces heat transfer and creates a corrosive environment.

To continuously monitor magnetite buildup, the Ames Lab team is proposing a built-in eddy current sensor. Essentially, EC sensors work by using a probe made of a wire coil. An alternating current passing through the probe generates a magnetic field around it. The probe's changing magnetic field generates current flow, or eddy currents, in the material. In turn, the eddy currents produce their own magnetic fields that generate reaction voltages in the coil. The resulting changes in coil impedance can be measured to gather information about the test material.

EC sensors can be made tough enough to survive the elevated temperatures and radiation found inside a nuclear reactor. For steam generator inspections, Ames Lab researchers are proposing a system in which an EC coil encircles tubes to provide a way to detect potential magnetite deposits inside the tube. One coil might even be able to monitor several tubes inside of it.

Use the force

Another critical inspection job is determining the structural integrity of steam generator tubes, especially where the tubes are attached to key support points, often by welding. For these areas, the researchers are studying ultrasonic testing using an electromagnetic acoustic transducer. Basically, an EMAT generates a static magnetic field and an alternating electric field inside the test piece placed nearby. The resulting Lorentz force acting on the test material generates sound waves that travel some distance. At the receiving end, these sound waves, in combination with the magnetic field, produce an electrical voltage that can be measured to provide information about the test material condition.

Unlike the more familiar type of ultrasonic testing used in medical applications — in which the sensor is coupled with the body via a thin layer of fluid or jelly — EMAT ultrasonic testing does not require that the sensor and sample be in contact. That, and the ability for EMATs to withstand high temperatures and radiation, makes EMAT UT an ideal NDE technology for nuclear power plants.

Moreover, EMAT UT can be used to send an acoustic wave, called a guided wave, down a tube to inspect its entire length. "Hopefully, our studies will tell us whether or not we can actually make a wave travel as far as needed, about 10 meters," says Nakagawa. The researchers are also exploring the use of EMAT UT for monitoring the reactor pressure vessel for cracking.

On-chip detectors

Another area under study is how to better monitor radiation levels in the reactor core by using radiation detectors, one more proven NDE technology. The technology may be used to monitor reactor fuel activities and perhaps other critical events.

The concept relies on new semiconductor-based radiation sensors. These on-chip detectors, about one-fourth the size of a dime, can withstand the high temperatures and radiation found in a nuclear reactor. The researchers are creating models to estimate gamma ray radiation intensities as functions of locations over the reactor life to determine how to best use these detectors. ◆

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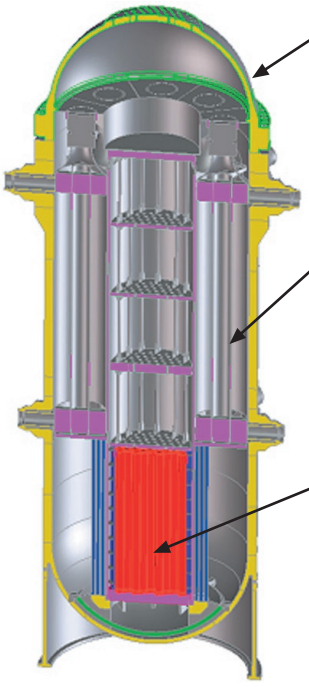
On-Line Monitoring for Safe Nuclear Power



Reactor Pressure Vessel	
Monitoring Need	*NDE Method*
Cracking	EMAT UT

Steam Generator	
Monitoring Need	*NDE Method*
Magnetite Deposits (Inside Tubes)	EC, EMAT UT
Tube/Tube Sheet Integrity	EMAT UT
Tube Integrity	EC, EMAT UT

Reactor Core	
Monitoring Need	*NDE Method*
Reactor core integrity, fuel activity anomalies, and fuel rod integrity	Gamma Ray Radiography

EC – Eddy Current
EMAT UT – Electromagnetic Acoustic Transducer Ultrasonic Testing

Ames Laboratory researchers have introduced the concept of on-line sensors to monitor the integrity of the next generation of nuclear power systems. These concepts, which use nondestructive evaluation methods, are being made available to designers of the advanced reactors (one of them is shown here).

It's All In the GAMESS

Chemistry code unravels molecular mysteries

by Saren Johnston

Mark Gordon (pointing) discusses GAMESS and other projects underway in the Scalable Computing Lab with Secretary of Energy Spencer Abraham when the Secretary visited Ames Laboratory's booth at Supercomputing 2002 in Baltimore.

What molecules do and why they do it is largely an enigma, a puzzle of giant proportions. But when all is said and done, it's molecular events that, simply put, make up the days of our lives. So it's not surprising that scientists continue to search for the reasons governing the actions and reactions of these mighty bits of matter.

Among those who are looking for answers to problems relating to molecules is Mark Gordon, Ames Laboratory program director of Applied Mathematics and Computational Sciences and head of Ames Lab's Scalable Computing Lab. Odds are Gordon may be having better luck at the search than others, luck being somewhat of a misnomer as it implies a certain degree of chance, and Gordon has not left this investigation to the game of chance.

No games, just GAMESS

Gordon and his Ames Laboratory coworkers are fostering and expanding a computational chemistry code that provides extensive and detailed information about how things work on the molecular scale.

The General Atomic and Molecular Electronic Structure System, known as GAMESS, includes a hierarchy of quantum chemistry methods that helps solve problems relating to molecules, making possible the design of new fuels and optical materials and the development of coatings that are resistant to extreme environments.

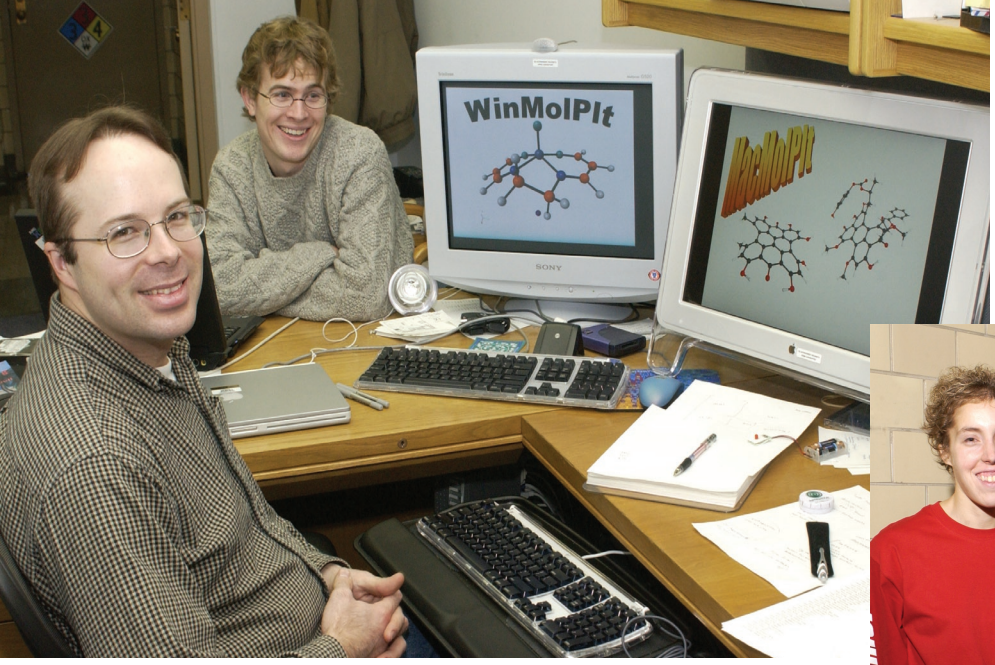
"All of chemistry, which also means all of biology, fundamentally involves molecular processes — that is, the way molecules react or behave," says Gordon, who is also an Iowa State University Distinguished Professor of Chemistry. "Chemistry, biochemistry, biology, materials science, physics — all ultimately can be reduced to what molecules do and why they do it. GAMESS allows you to answer those questions."

Using GAMESS, Gordon, his co-workers and the students in his research group are making major contributions to the design of new rocket fuels for the Air Force. "We're also involved in a Grand Challenge program for the Department of Defense, using GAMESS to help design new optical materials, fuels and wear-resistant coatings," says Gordon. "Some of my former students are now using GAMESS to study biological processes, such as protein behavior."

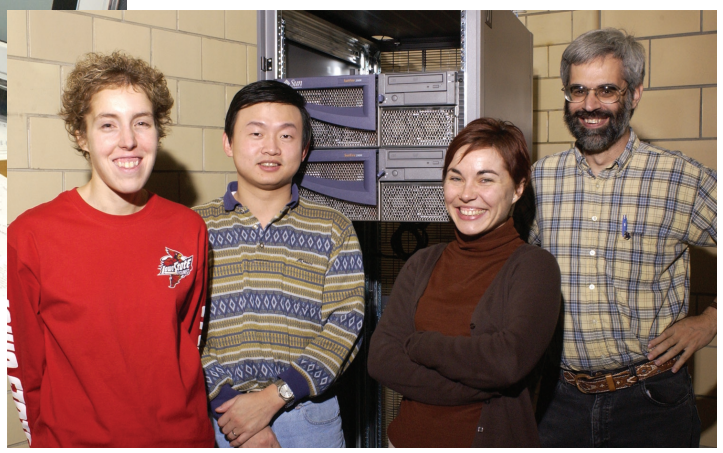
Historically speaking

The history of GAMESS goes back to 1977 when the initial version of the code was assembled, under the direction of Dr. Michael Dupuis, from several existing quantum chemistry computer programs by the staff at the National Resource for Computations in Chemistry. The original project was funded by the National Science Foundation and the Department of Energy from 1977 to 1981. However, the continued development of GAMESS from 1982 to present is directly due to the funding provided by the Air Force Office of Scientific Research; to the nurturing environment provided by Gordon; and to the expertise demonstrated by Gordon, Ames Lab associate Michael Schmidt and many students and postdoctoral fellows in developing new functionalities and parallelizing the code. Making a code operate efficiently in parallel refers to organizing it so that it can take advantage of parallel computers — those with several processors that can work on different parts of a single problem simultaneously. Also, contributions to the GAMESS program from Gordon's many colleagues and from students who have been in his research group have added tremendously to the current robust nature of the code.

"GAMESS is what's called a legacy code," says Gordon. "It existed far before anything of its kind, so some features of GAMESS have been made parallel from the beginning, and some features have been made parallel after the fact. I've always had at least two or three students and postdocs specifically working on how to make GAMESS more parallel," he says. "It's our forte — what we like to do is develop these very sophisticated methods, in many cases with colleagues, and make them parallel and more efficient so we can apply them to bigger molecular systems. It's something we do better than most." A major result of this ongoing effort



Brett Bode (foreground) and Ryan Olson bring the results of complicated GAMESS calculations to life through their respective visualization programs, MacMolPlt and WinMolPlt.



Members of the Gordon group working on GAMESS enhancements are, left to right, Heather Netzloff, Jie Song, Ivana Adamovic and Michael Schmidt. The researchers will make good use of the two Sun systems pictured behind them in developing new GAMESS techniques.

by the Gordon group is that an increasing percentage of the features in GAMESS, especially the most computationally demanding ones, can be done in parallel.

Supplementing the software suite

In addition to excelling at writing parallel code for GAMESS, Gordon and his Ames Lab collaborators, Schmidt and Klaus Ruedenberg, who is also an ISU Distinguished Professor of Chemistry, are particularly adept at creating sophisticated and complex methods for the software suite that address unusual chemical species.

"When you have chemical reactions going on, especially under severe conditions, such as high temperature or high pressure, you encounter chemical species that you would not even call molecules," Gordon explains. "These are things that don't hang around very long, and you may never see them. They're intermediates and may have lifetimes of only picoseconds or femtoseconds, but they may be very important in the overall reaction process. One of our goals is to develop methods to treat these very unusual species, and the more nontraditional the method, the harder it is to make parallel."

An innovative research tool, GAMESS includes a novel graphics visualization program, MacMolPlt, written for Macintosh computers by Ames Lab associate scientist, Brett Bode. Gordon says MacMolPlt eases the task of interpreting the various complicated calculations performed by GAMESS. Ryan Olson, a graduate student in Gordon's group, is developing WinMolPlt, a Windows version of MacMolPlt. "Ryan has half a dozen people around the world testing this program, so now you can visualize the results of GAMESS calculations if you have a Mac or a PC," says Gordon.

A unique feature of GAMESS is the effective fragment potential, or EFP, which was initially developed by Gordon and Jan Jensen, a former graduate student of Gordon's now at the University of Iowa, in collaboration with Dr. Walter Stevens and his group at the National Institute of Standards and Technology. Stevens is now director of the DOE Chemical Sciences Program. Over the past decade, several graduate students and postdoctoral fellows working with Gordon have contributed to the development of the EFP method, including current students Heather Netzloff and Ivana Adamovic and postdoctoral associate Jie Song.

"Sometimes scientists deal with systems in which there are so many atoms and electrons that quantum mechanics can't be done, even at simple levels," says Gordon. The EFP method is based on quantum mechanics, but it's not quantum mechanics — it's a simple but sophisticated model potential that represents most of the quantum mechanics effects at a very reduced computational effort. The EFP method can be combined with actual quantum mechanics in such a way that a quantum mechanical description is required only in that part of a chemical system that is undergoing a chemical change. The remainder of the system is treated with EFPs, so that the entire calculation takes orders of magnitude less computer time than a fully quantum calculation.

"The EFP is a sophisticated model to predict how solvents effect chemical reactions and to predict the behavior of liquids," says Gordon, "and it's working very well.

GAMESS offers an amalgam of choices for quantum mechanical modeling of molecular systems. As such, it proves to be an indispensable tool for today's chemical researchers who have the benefit and availability of increasing computational power to probe the molecular world. Evidence of its capabilities is the fact that GAMESS is used at well over 5,000 sites worldwide, ranging from high schools and research universities in the United States and abroad to government laboratories and the private sector. And best of all, GAMESS is distributed at no cost to users by accessing *www.msg.ameslab.gov* and signing a license agreement. ◆

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Shattering
Intermetallic Conventions

by Kerry Gibson

Ames Laboratory researchers identify non-brittle intermetallic compounds

Ames Laboratory senior metallurgist Karl Gschneidner, Jr. demonstrates the ductility of a "button" of yttrium-silver (YAg). Unlike most intermetallic materials that are quite brittle at room temperature, Gschneidner and a group of Ames Lab researchers have identified more than a dozen rare earth/main group metal (RM) intermetallic compounds that show high levels of ductility and toughness.

Scientists have known for more than 100 years that intermetallic materials — compounds consisting of two or more metals bonded together — possess chemical, physical, electrical, magnetic, and mechanical properties that are often superior to ordinary metals. The problem with these promising materials is that they're quite brittle at room temperature. Until now.

Ames Laboratory researchers have discovered a number of rare earth intermetallic compounds that are ductile at room temperature. The discovery, to be announced in an article in an upcoming issue of the journal *Nature Materials,* has the potential to make these promising materials more useful.

Brittle is the rule

"Many intermetallic materials are too brittle to handle," says Ames Laboratory senior metallurgist Karl Gschneidner, Jr. "If you drop them, they shatter. But you can beat on these new materials with a hammer, and they won't shatter or fracture … they're that ductile."

So far, the Ames Laboratory research team led by Gschneidner and materials scientist Alan Russell has identified 12 fully ordered, completely stoichiometric intermetallic compounds. In other words, these materials are combined in the proper chemical ratios and the atoms are properly lined up.

"Intermetallics have been studied for decades," Russell said. "Tens of thousands of them have been identified, and there's a whole menu of 'tricks' that can be used, such as testing them at high temperatures, in zero-humidity, or shifting them off stoichiometry, to make them somewhat ductile. The materials we're studying are the first ones that don't need these contrivances."

B2 structure key?

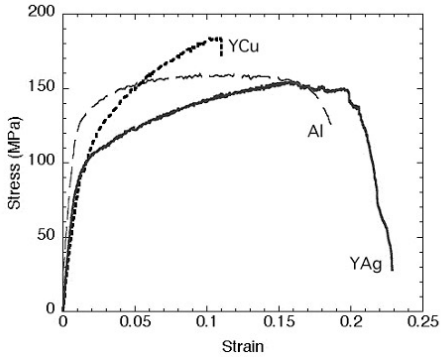
By combining a rare-earth element with certain main group or transition metals, the resulting binary compound has a B2 crystal structure. That alpha-numeric designation, developed by crystallographers, means that the compound has a crystal structure like that found in cesium-chloride (CsCl) in which an atom of one element is surrounded by a cubic arrangement of eight atoms of the other element.

The study has focused on yttrium-silver (YAg), yttrium-copper (YCu), and dysprosium-copper (DyCu), but a preliminary examination of other rare-earth compounds showed that cerium-silver (CeAg), erbium-silver (ErAg), erbium-gold (ErAu), erbium-copper (ErCu), erbium-iridium (ErIr), holmium-copper (HoCu), neodymium-silver (NdAg), yttrium-indium (YIn), and yttrium-rhodium (YRh) are also ductile.

In tensile testing, these materials showed remarkable ductility. The YAg stretched nearly 25 percent before it fractured, compared to 1 percent or less for many other intermetallics. In other measurements, the materials showed fracture toughness values comparable with commercial aircraft aluminum alloys.

Why these materials deform while other intermetallics shatter isn't quite clear, but theoretical calculations by Ames Lab physicist James Morris show that the ductile materials possess much lower unstable stacking-fault energies that exist around defects in the crystal structure of the materials. Because these energies are lower in the ductile materials, it may be easier for them to plastically deform instead of fracturing at the grain boundaries.

"There are particular planes (within the B2 structure) that tend to slip most easily," Russell says, "and particular directions on those planes where deformation slip occurs most easily. However, we have transmission electron micrographs that identify slippage in a direction we didn't see in our single crystal studies, so there are probably other factors at work as well."



Tensil stress-strain properties of polycrystalline YAg (solid curve) and YCu (short-dash curve) tested in air at 22 C compared with commercial 3105 aluminium alloy (long-dash curve).

Exceptional understanding

While there may be applications for these ductile materials because of their other characteristics, such as high-temperature strength or corrosion resistance, Gschneidner and Russell hope that studying these materials will actually lead to a better understanding of the brittle intermetallics.

"The most exciting thing about them is when they break all the rules like this, it gives you a great opportunity to figure out fundamentally why the others are brittle," Russell says. "To see one that's the exception gives you a new perspective on all the others."

Gschneidner adds, "The exceptions are the ones you want to concentrate on because they can tell you a heck of a lot more than all the ones that obey the rules. It can steer you in a whole new direction and lead to one of those 'eureka' moments."

Since the discovery of these materials evolved from work on another project, it has received only minimal funding. Gschneidner has pursued it as one of his interest areas with the other team members "volunteering" hundreds of hours of their time. In addition to Gschneidner, Russell and Morris, the team includes materials scientists Alexandra Pecharsky and Josh Zhang, senior metallurgist Tom Lograsso, nondestructive evaluation researchers David Hsu and Chester Lo, visiting physicist Ye Yizing, and students David Kesse and Aaron Slager. Physicist and Ames Laboratory deputy director Bruce Harmon and metallurgist Bulent Biner were also involved in theoretical discussions of the materials.

Overall, Russell calls the amount of knowledge gained per dollar spent "absolutely staggering." However, the group has submitted a funding proposal for further research to DOE and has filed a patent application for the materials. ◆

The yttrium-silver button shows dents and deformation from repeated hammer blows. The gadolinium-silicon-germanium material was shattered with a light tap from the hammer.

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The Best *Reality Show* Around

Searching for the ultimate reality, researchers are investigating the quantum world

by Saren Johnston

If "all the world's a stage," as Shakespeare wrote in *As You Like It,* then we might logically ask, what's going on behind the scenes? What's directing or orchestrating that daily, worldwide grand performance?

A theoretical physicist might say this scenario represents a good way to think about classical and quantum physics. Classical physics describes the world we see — the stage — with all the players, objects and activities we encounter daily. It includes everything from the life-saving Mr. Coffee machine we switch on in the morning to the welcoming bed we gratefully crawl into at night, and all things in between. Classical physics is concerned with matter and energy on an observable scale.

Quantum physics, on the other hand, explains the nature and behavior of matter and energy in the worlds we can't see — the atomic and subatomic worlds "backstage," if you will. It deals with discrete, individual units called "quanta" that interact with their entire environment and allow a more explicit description of the exact nature of reality. In the quantum mechanical world, it is possible for a particle, such as an electron, to be in two or more different quantum states at the same time. Although the atomic world described by quantum mechanics is nothing like the world we live in, it presides over that world — its sets and cast of characters.

Considering the existence of both a classical and quantum mechanical world, it's only natural to wonder what happens when the two meet. At what point does the quantum mechanical world end and the classical world begin, and how does that happen? The issue is one that intrigues Ames Laboratory associate physicist Viatcheslav Dobrovitski.

Viatcheslav Dobrovitski's home is a world away in Russia. But even at that great distance, it's more accessible than the quantum world that draws the young physicist's attention. To investigate that hazy, indistinct world, he uses supercomputers to simulate the behavior of quantum states in specific environments, a research effort fundamental to the successful development and operation of quantum computers.

"In quantum mechanics, all the objects we know are not localized in space, but have some spread," says Dobrovitski. "They are cloudy and uncertain. So, there is the problem of trying to connect the quantum mechanical world and our local and relatively certain everyday world. Many objects that at first sight look essentially quantum mechanical, are not," he says. "They can be explained in terms of classical statistical mechanics. But there are some very special states that cannot be explained from this point of view. These states are quantum mechanical when the system is small, but their properties make them classical when the system becomes sufficiently large."

Dobrovitski notes that what he and his Ames Laboratory co-workers are trying to do is half science and half education. "It's the education of ourselves and, hopefully, of other people to try to understand which states in a system are intrinsically quantum and which are, in fact, classical. The problem is that all true quantum mechanical states are strongly entangled."

It takes two to "tangle"

Quantum particles that have interacted with each other can exist in pairs in an entangled state — a superposition of states that ceases to exist when some physical property, such as spin, is measured. (Spin is the intrinsic angular momentum of a nucleus or an elementary particle, such as an electron.) Entangled quantum particles will retain some type of connection, even when separated by great distances — "spooky action at a distance" is how Einstein described it. The relationship develops because the two particles occupy a joint quantum state and move coherently with

one another. Quantum entanglement is a phenomenon that has been demonstrated through experiments time and again. It is essential to the emerging field of quantum computing, allowing individual quantum bits, or qubits, to interact with each other immediately, yielding enormous gains in time and memory for some algorithms.

"Spin City"

"Many quantum states are self-destructive," says Dobrovitski. "They decay into a mixture of two classical states, with the outcome remaining classical in one state or the other." That outcome might be triggered by the quantum state interacting with an environment of nuclear spins that are present in the system. Offering a magnetic molecule as an example of a classical system, Dobrovitski says it has only two possible choices of where to direct its spin — wholly up or down. However, when the system was quantum mechanical — that is, before coherence of different states was destroyed — there could be all possible superpositions of the spin state. Up, down, or any superposition of the two is allowable.

"In the process of a measurement, the system must 'choose' the way the spin will be directed, and how it chooses this is an unsolved problem," says Dobrovitski. "It's very amazing that a truly quantum mechanical system behaving in a quantum mechanical way becomes a classical system with choice — a system that can be described by statistical physics. And now, of course, the problem is to understand how this choice is made."

What a state we're in!

"All right," said the Cat; and this time it vanished quite slowly, beginning with the end of the tail, and ending with the grin, which remained some time after the rest of it had gone."

~ Lewis Carroll
Alice's Adventures in Wonderland

Dobrovitski's research has shown that some of the coherences in entangled pairs are less stable than others in respect to interactions with the environment. "The transition from quantum to classical is not a simple matter," he says. "We know now that this transition is associated with stealing some coherences."

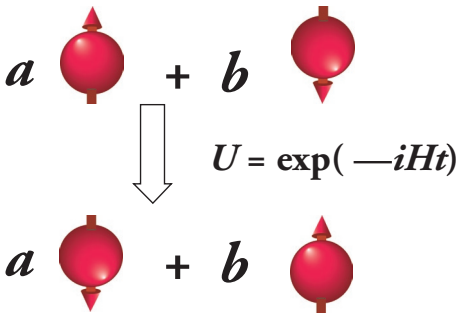
In their research efforts to add to the knowledge base about how a quantum mechanical system becomes a classical system with choice, Dobrovitski and his co-workers are investigating quantum oscillations. "Many people believe quantum oscillations are intrinsically quantum," he says, "but in a sense, they are not. They belong to this category of classical system with choice."

Dobrovitski has discovered that in some cases quantum oscillations can be seen in decohered, nearly classical systems — those in which nearly all coherence has been destroyed between any pair of entangled particles. "The remaining quantum part will exhibit quantum phenomena. As a whole, the system is no longer quantum, but it still remembers something of its quantum legacy well into the future, until it becomes totally classic," he explains.

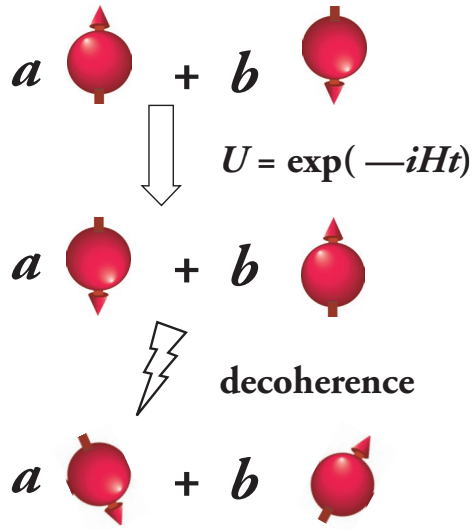
"It is a big problem to clearly sort out all the phenomena we encounter in the transition from quantum to classical with choice," says Dobrovitski. "We have some understanding of how it happens, but we need to clarify how various systems behave in different situations."

He adds that the research is intriguing from both the basic and applied points of view. "On one hand, it's interesting from the aspect of the fundamental understanding of the quantum measurement problem," he says. "The other thing is that it might hold some interest for quantum computing, because this transition from quantum to classical is probably the main thing that jeopardizes quantum computations."

Dobrovitski notes that although some very small-scale quantum computing has already been implemented in quite a few systems, the self-destructive nature of quantum mechanical states interacting with the environment — decoherence — is a huge problem. "They decay very fast, so the idea is to understand what determines this rate of decay and if we can slow it down to where more than just a few quantum computational steps can be performed," he says. Such a feat would be a significant accomplishment, making possible the potential construction of modest-size quantum computers that would allow certain types of calculations to be performed, such as the factorization of large numbers. And massive calculations of this kind are far beyond the capabilities of any classical supercomputer. ◆



This figure represents the ideal, but elusive, scenario for a quantum computer. The quantum bits, or qubits, are represented by spins that are interacting coherently with one another with no disruption from the surrounding environment.



This figure represents the real-life scenario for a quantum computer. The coherence of the interacting qubits is quickly destroyed, or decohered, by disturbances from the surrounding environment, such as neighboring nuclear spins or lattice vibrations. This loss of coherence, or transition from quantum to classical, leads to a rapid generation of errors and is the biggest roadblock to quantum computations.

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Making Their Mark in Forensics

by Steve Karsjen

Stan Bajic looks at an image of a toolmark embedded in the surface of an ordinary pair of pliers. A forensic comparison microscope is used to capture digital images of toolmarks, which are being entered into a database. Forensic experts can use the database to identify toolmarks produced through different manufacturing processes.

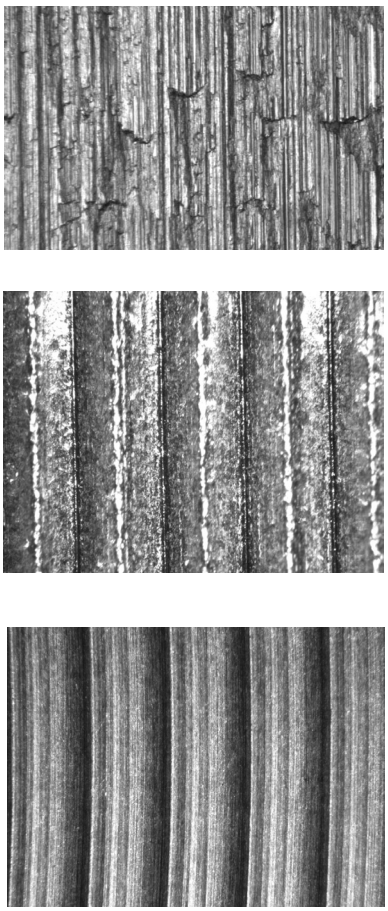
Astronomical — that's the term DNA investigators put on the chances of the DNA of one person matching that of another. In fact, some estimates place the odds that two people will have the same DNA at 200 billion to one. It's a certainty level that all but assures that when DNA evidence is introduced in criminal cases, the criminals are likely to land in jail.

What if the statistical certainty the courts rely upon when accepting DNA evidence was also available at some level for matching weapons found on suspects to the crimes? Unfortunately, at this time there is no scientific way of indisputably proving in the courts that a tool, such as a screwdriver found on a suspect, was the actual tool used to perpetrate the crime. However, the future might tell a different story thanks to two separate, but complementary, research projects underway at Ames Laboratory. Both projects are attempting to help forensics experts make their case by examining the uniqueness of toolmarks.

It's all in the marks

As one might imagine, there are many commercial tool-manufacturing companies, both in this country and abroad. Probably not as well known in the general community, but certainly well known in the forensics community, is that during the manufacturing process and through normal use, tools, such as screwdrivers, pliers or wire cutters, are left with certain marks, or imperfections, embedded on their surfaces. These patterns are believed to make each tool unique.

An interesting fact about toolmark identification is that when tools are used to perpetrate a crime, such as jimmying a door, the patterns on the tools are transferred to the crime scene. In the past, forensic investigators would take a tool found on a suspect and visually examine scratches made with that tool in the lab to scratches on objects from a crime scene. Through this visual examination of the toolmarks from the tool and on the crime-scene material, they would attempt to match the tool to the crime. If the scratch patterns matched, the



Images (above) show the types of toolmarks that can be created during the manufacturing process. The first example (top) shows toolmarks resulting from broaching; the second, broaching followed by laser hardening; and the third, milling.

investigator had a case. If not, he or she didn't. It all sounds very straightforward. And for some time, it was. But recently the waters have been muddied in the courts.

This traditional qualitative approach used by forensic investigators, which is based on years of experience in forensic examination, was recently challenged in a case before the Florida Supreme Court (Ramirez vs. State of Florida, 2000) and resulted in a critical toolmark match being deemed inadmissible as evidence. Essentially, the court claimed that the "proposition of uniqueness" for tools based on toolmarks was a scientific theory that has been inadequately tested by the scientific community.

"In essence, testimony introduced has to be proven by scientific method," says Scott Chumbley, an Ames Laboratory metallurgist and Iowa State University professor of materials science and engineering, who is working on one of the new methods that may help address the Supreme Court's requirements for quantification in toolmark identification. Currently, there is no concrete evidence out there, nothing in the literature to prove tools and their marks are unique based on certain manufacturing processes, say both Stan Bajic, Ames Laboratory associate scientist, and David Baldwin, director of the Laboratory's Midwest Forensics Resource Center, co-principle investigators on the toolmark identification project.

The sum of its parts

Bajic's research is a two-fold project. The first part involves building a database of toolmark images. The unique database consists of digital images of the striations on the surfaces of tools that are produced by six different manufacturing processes: filing, grinding, milling, whetstoning, broaching and stamping.

The Ames Lab database is the first to incorporate numerous manufacturing methods and so many samples. Past studies of these manufacturing processes have been done but were limited in the number of samples used (less than 10 per study). Bajic says building the database will require the production of multiple images through the use of a forensic comparison microscope equipped with a charge-coupled device camera.

To date, the collection of tools being imaged for inclusion in the database includes screwdrivers, pliers, wire cutters, bolt cutters, tin snips, cold chisels, wood chisels and pry bars — tools that have been acquired directly from commercial manufacturing companies.

In addition, steel blanks have been acquired and processed in the Ames Laboratory machine shop to produce additional, more controlled, toolmark samples of the various manufacturing processes. Bajic says having both commercial and shop-made sample sets will provide a large collection of sample sets for determining comparison criteria for each manufacturing process and yield a statistical basis for toolmark comparison.

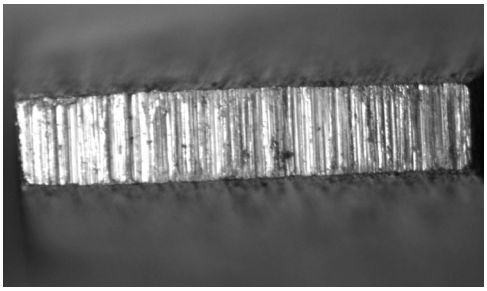
Originally, Bajic and graduate students Amber Umble and Molly Schiel planned to take images of 100 sets of tools for each of the six manufacturing processes. However, each tool presents more than one machined surface, so as many as four sets of images were collected for each tool. So what started out to be 100 images quickly turned into 400 images. And after they took into account the fact that it was necessary to include multiple magnifications and replicates for each image, the number grew to more than 1,000 images per set of tools. "Right now we have over 8,000 images and by the time this project is done, I imagine we'll have 13,000 images for all these tools," said Bajic.

Once Bajic has all the digital images in the database, the second phase of the research project will kick in. The images will be used to produce a software tool for the reduction and analysis of the image data. Algorithms will be developed and used for the comparison of the various toolmarks.

Creation of the software is being spearheaded by Max Morris, a professor in the Iowa State University statistics department. Morris, who is also a professor of industrial engineering at ISU and an Ames Laboratory associate, describes how the software will be used in the following way. Normally a forensics expert will take the samples (one from the crime scene and the other from the tool) and put them under a microscope. Then the expert will move them around and, based on years of experience, will try to line them up and find a point at which they meld together enough to be called a match.

Morris has actually watched Jim Kreiser,

Tin snips are just one of the tools whose surfaces are being imaged for a toolmark database.



A digital image of the tip of a screwdriver dramatically demonstrates the uniqueness of toolmarks created during grinding, one of the many manufacturing processes used to produce tools.

a retired toolmark examiner with over 34 years with the Illinois State Police Forensic Science Laboratory system, do this in the lab. "We've taken notes and asked questions and have come back and started dealing with how we take the digital images provided by the database apart and mimic the process the examiner goes through.

The idea is to do substantially what he does with bits of pixels instead of the actual image on the microscope," says Morris. And thus far he says the experiment has been a success. He and graduate student Zhigang Zhou have developed an image-analysis algorithm that works on a very small set of test images. "Basically our preliminary results have been perfect," says Morris. "Every time we should get a match between two images, it clearly comes up with a high degree of similarity. And when we shouldn't get a match, when the images are of different items, the index is much, much lower."

Morris is quick to point out that even though the algorithm can mimic the behavior of forensic examiners, it will never replace what they do because there are subtleties in what real toolmark examiners do that have taken a lifetime of experience and knowledge to develop.

"We could never build all that into an algorithm," says Morris. "The best we can hope for is that the algorithm would be a type of first-order approximation for the toolmark examiner. We're hoping to be able to do a separation of the obvious stuff very quickly so that the toolmark examiner can focus his energy on the more complicated cases to call," he adds.

Ultimately, Bajic hopes the work he and Morris are doing will culminate in the statistical tools necessary for validation of the proposition that particular manufacturing methods produce marks on tools that are substantially different from tool to tool. "In the end, what we will be trying to say, for example, is that the chances of this screwdriver having the same marks as another from the hardware store are one in 10,000 or some number. That's what we want this tool to do — provide that probability prediction," says Bajic.

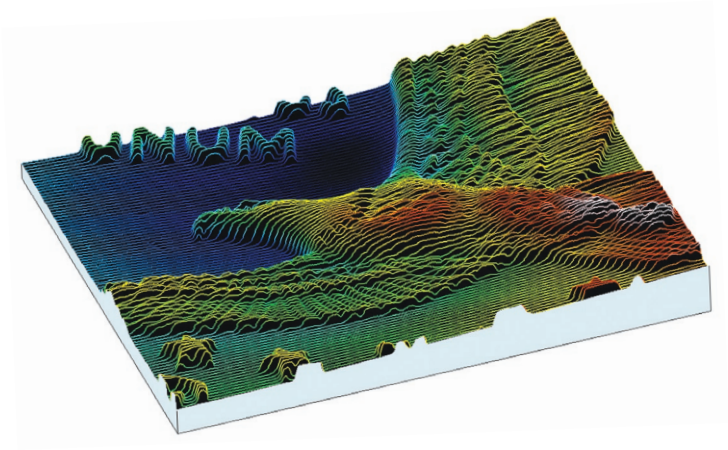
Morris admits that there is a lot of interest in providing the probability prediction Bajic talks about, especially on the part of the FBI, which is funding the research. But right now he cautions that the software is far from being able to do that on a large scale because of the variation in the way tools are produced by manufacturers. "What we are developing is a set of tools that can work in the tightly controlled, narrow artificial population that we're setting up with this database." he adds. "It's an important first step."

Jumping a dimension

Stepping from a two-dimensional to three-dimensional look at toolmarks is the goal of Chumbley's research. He and co-principal investigator Larry Genalo are using 3-D characterization methods and statistical methods to identify toolmarks. Their research involves using a profilometer, a scanning tool that measures the height or depth of toolmarks and then develops a type of contour map of the marks from the scan. This map can then be used to precisely identify a toolmark, allowing forensic specialists to match the mark on the tool to the tool manufacturer.

Like Bajic's work, this scientifically tested technique may also one day address the needs of the court system for providing quantifiable scientific data with known measures of reliability. Preliminary results show the reproducibility of the instrument is better than 99.9 percent on known samples.

"It's a pretty good fit," announced Chumbley during a presentation at the Midwest Forensic Resource Center's annual meeting in June at Ames Laboratory. The



This image of an American Eagle on a Sacagawea dollar resulted from a scan by a profilometer. The scan is used to create a contour map that illustrates the detail and resolution that can be produced by the instrument.

MFRC consists of crime laboratory officials from across the Midwest, and Chumbley's research project is one of five projects currently being funded by the MFRC at the Ames Lab and Iowa State. One of those attending the MFRC meeting was Mike Stone, a member of the Omaha Police Department's crime laboratory, who perhaps best summarized the criticality of all of the toolmark research underway at the Ames Laboratory. Reacting to Chumbley's presentation, Stone said, "This research has great application to my world. Everything we do is geared toward the discovery and identification of evidence." ◆

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INtouch

A Visit from the Secretary

"A nation that embraces basic research embraces a brighter future," said Secretary of Energy Spencer Abraham speaking at the all-hands meeting of employees during his 2002 visit to Ames Laboratory. The Secretary had come to the Lab to formally recognize and open the Midwest Forensics Resource Center, a facility that serves the needs of regional crime labs and expands the capabilities of forensic science.

Time and again throughout the all-hands meeting Secretary Abraham emphasized the importance and value of basic research to the Department of Energy's mission of ensuring national security. "In my view, a serious commitment to national security demands a serious commitment to science, including basic research," he said. "This commitment strengthens our energy security, international competitiveness, economic growth and intellectual leadership."

Congressman Tom Latham accompanied the Secretary on his visit to Ames Lab. Latham was able to secure $3 million in funding to help establish the MFRC, which is directed by David Baldwin, who also directs the Lab's Environmental and Protection Sciences Program.

During the Secretary's brief visit, he met with three of the Lab's R&D 100 Award-winning scientists: Ed Yeung, John McClelland and Iver Anderson. Each scientist introduced the Secretary to his individual research efforts, two relating to forensics investigations and homeland security and another highlighting metallurgical techniques that contribute to the Lab's continuing status as one of the world's premier materials science labs.

Concluding his remarks at the all-hands meeting, Secretary Abraham said, "I'm very proud to be the Secretary of Energy and have the chance to work with people like yourselves. At the end of the day, it's only the men and women in the front lines who make the breakthroughs, who bring their talent, curiosity and skill to translate that research work into remarkable achievements like those that have been undertaken here." ◆

Secretary of Energy Spencer Abraham (left center) and U.S. Rep. Tom Latham (right center) join Ames Laboratory Director Tom Barton (far right) and Iowa State University President Gregory Geoffroy (far left) prior to the Secretary's all-hands meeting with Lab employees.

Research technician Arne Swanson holds an ingot of material that was consolidated in the bright blue Retech 150 plasma furnace, shown behind him in the Materials Preparation Center.

New Furnace a Real "Hot Shot"

Ames Laboratory's Materials Preparation Center has a new, powerful tool in its arsenal that even the toughest alloys can't withstand. Capable of generating temperatures in excess of 10,000 degrees Celsius, the Retech Model 150 Plasma Lab Furnace will melt about anything.

"There's no limit to the metals or metal alloys it can melt," says MPC director Larry Jones. "We are using it primarily for melting reactive metal alloys, but it gives us enhanced capabilities in other areas as well."

One of the advantages of the furnace is that reactive metal alloys can be melted without the need for a crucible. "Some materials can't be melted in a typical crucible furnace because they react with the crucible material, contaminating the molten metal," Jones says. "This new furnace doesn't require such crucibles, so we eliminate that problem.

Instead, the metal alloy is hydraulically pushed into the chamber by a bar feeder. The plasma torch moves back and forth across the end of the bars as they stick out over a water-cooled, thick copper mold."

Even though copper has a lower melting temperature than many metals, it is used for molds because it conducts heat so well. Heat is transferred so quickly to the cooling water that the molten metal cools, solidifies and shrinks away from the surface of the copper before the copper melts. The mold forms the melted material into an ingot.

The heart of the furnace is a plasma torch that uses a helium and argon mixture as the feed gas. The plasma torch works by injecting the feed gas into a hollow electrode. The gas then carries an electrical arc from the electrode through a nozzle and to the grounded workpiece. The electrical discharges add energy to the gases in order to increase the gas temperature beyond that normally attainable by chemical reaction.

One of the initial tasks for the furnace has been to consolidate material, turning multiple pieces of long metal bar stock or piles of granular material into short, stout ingots. This dramatically reduces the overall surface area and lessens the amount of surface oxidation that takes place while the metals are being stored for future use.

"Beyond that, we can do any number of things when it comes to melting and reforming materials," Jones says, "and it's just one more capability we have to meet the research needs of our scientists." ◆

Barton Named FLC Laboratory Director of the Year

Since 1999, the Federal Laboratory Consortium has been honoring outstanding Laboratory directors with its Laboratory Director of the Year award. One of this year's recipients is Tom Barton, director of the Ames Laboratory.

The Laboratory Director of the Year award is given annually to directors who have made outstanding contributions supporting technology transfer activities at their laboratory. Barton received the award on May 7, 2003, at the FLC National Meeting in Tucson, Ariz.

"It's an honor to be recognized by the FLC because this organization represents the best in efforts to help federal laboratories, such as Ames Laboratory, strengthen ties with industry," Barton said. "These ties are essential if we are to help build Iowa's and our nation's economy."

Ric Trotta (left), Chair of the FLC Advisory Council, presents a plaque to Tom Barton recognizing him as a Federal Laboratory Consortium Laboratory Director of the Year.

Iowa State University President Greg Geoffroy congratulated Tom Barton in a letter of recognition:

"Congratulations on the very good news that the Federal Laboratory Consortium for Technology Transfer has named you Laboratory Director of the Year. You have worked tirelessly in shaping the focus of the Ames Laboratory and making sure that the Ames Lab is accessible to industry. Your efforts have succeeded in making the Lab a rich resource for Iowa business and industry, and you have helped, therefore, to generate needed economic growth for the state."

The FLC is a nationwide network of more than 700 federal laboratories and centers and their parent departments and agencies. The FLC's primary focus is moving federal laboratory research and technology into the mainstream of the U.S. economy. Each year, the FLC's awards committee receives nominations for director of the year from FLC members. The selection is made based on each nominee's ability to enhance technology transfer in economic development or apply research to technological advancements in the field.

"Because of the competitiveness and prestige of the award, being selected as a recipient is an honor which recognizes both the excellence of your efforts and your facility's technology transfer program," said Ann Rydalch, chair of the FLC, in a congratulatory message to Barton.

Barton has been director of the Ames Laboratory since 1988. The Laboratory's technology transfer program provides numerous opportunities for companies to collaborate with the Lab, from contract research to licensing of intellectual property.

"It makes you feel good to help a company," Barton added. "After all, they're paying for it. Their tax dollars pay for our work." Since 1986, 136 U.S. patents have been issued on technologies resulting from Ames Laboratory research. In addition, Laboratory research has been the basis for 14 start-up companies. The most recent of these is CombiSep Inc., which manufactures the MCE2000, a sophisticated instrument for separating and measuring a variety of chemical compounds.

This is not the first time Barton has been recognized by the FLC. In 1999, he was elected a member of the organization's National Advisors Group. This select panel of approximately 15 people provides guidance to the FLC in pursuing its technology-transfer goals and making the organization more effective. The group includes senior agency officials, laboratory administrators and industry leaders. As part of his award, Barton participated in the annual FLC Laboratory Directors' interactive forum, "Directing the Future," which took place the morning following the awards ceremony. ◆

L♥ve That Science Bowl!

Annual competition has huge following

None of us is too thrilled about giving up a Saturday for something that's not essential to our usually packed weekend agenda. But Science Bowl, well, that's another matter!

Annually, on the last Saturday in January, approximately 48 high school teams and 75 Ames Laboratory and Iowa State University volunteers take over every available room in Iowa State's Memorial Union to participate in the daylong science competition. Happily, no one seems to mind losing a little extra sleep on a Saturday morning, putting off household tasks, postponing study plans, or even missing Saturday morning cartoons to take part in the exhilarating event. And this year was no exception.

Forty-four Iowa high school teams showed up for the Jan. 25th competition. But it was Cedar Rapids Washington High School in Cedar Rapids, Iowa, that came from behind in the closing seconds of the championship match to win the 2003 Ames Laboratory/Iowa State University Regional High School Science Bowl. Washington won all 10 of its matches to advance to the U.S. Department of Energy's National Science Bowl, May 1-5, in Washington, D.C.

Many of the schools participate in Science Bowl year after year. "It's our favorite competition of the year," said Phyllis Bishop, Science Bowl coach from Chariton High School. "It's always so well planned and run in a very efficient manner."

Coach Rhonda Thompson of Decorah High School said, "Thank you for the Science Bowl experience. My team of rookies really enjoyed it, felt proud to have done O.K. against mostly older teams, and are already looking forward to next year."

Volunteers, too, find they enjoy the Science Bowl experience and the opportunity to interact with so many smart and gifted students. "Working with youth and promoting science education is one way I can 'pay back' for support I received," said Donald Lewis, an ISU entomology professor and a longtime Science Bowl volunteer. "Reading questions at Science Bowl helps keep me humble. These students are so bright and talented, and they know so much about so many different things. I am awed by their abilities and reminded of my own limitations."

Surprise, relief, exhilaration — Cedar Rapids Washington coach Heather Adams displays some of each emotion as her team wins the 2003 Ames Laboratory/ISU Science Bowl.

Although many of the people who volunteer for Science Bowl have scientific backgrounds, just as many don't. "There are tasks available for everyone, such as timekeeping and scorekeeping," said Ellen Price, an Ames Lab account specialist who just completed her third year as a timekeeper for the competition. "Since you don't have to be a scientist or need special skills to help, it's something I can do and it's also an opportunity to represent Ames Lab in a positive way. It's a fun and energetic atmosphere, and it's interesting to hear part of the competition and see all the high school teams that come to participate." ♥

"I can't believe I did that!" Perhaps Joe Hove, captain of the Solon High School team, forgot to wait until the moderator recognized him before giving his answer — a definite Science Bowl "no-no" as the question is then offered to the opposing team.

The Ames Laboratory/ISU Science Bowl winning team from Cedar Rapids Washington High School, left to right: Jeff Barnes, Ashley Noreuil, Jake Thomas, Krystal Garringer and Aaron McDowell.

INquiry

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