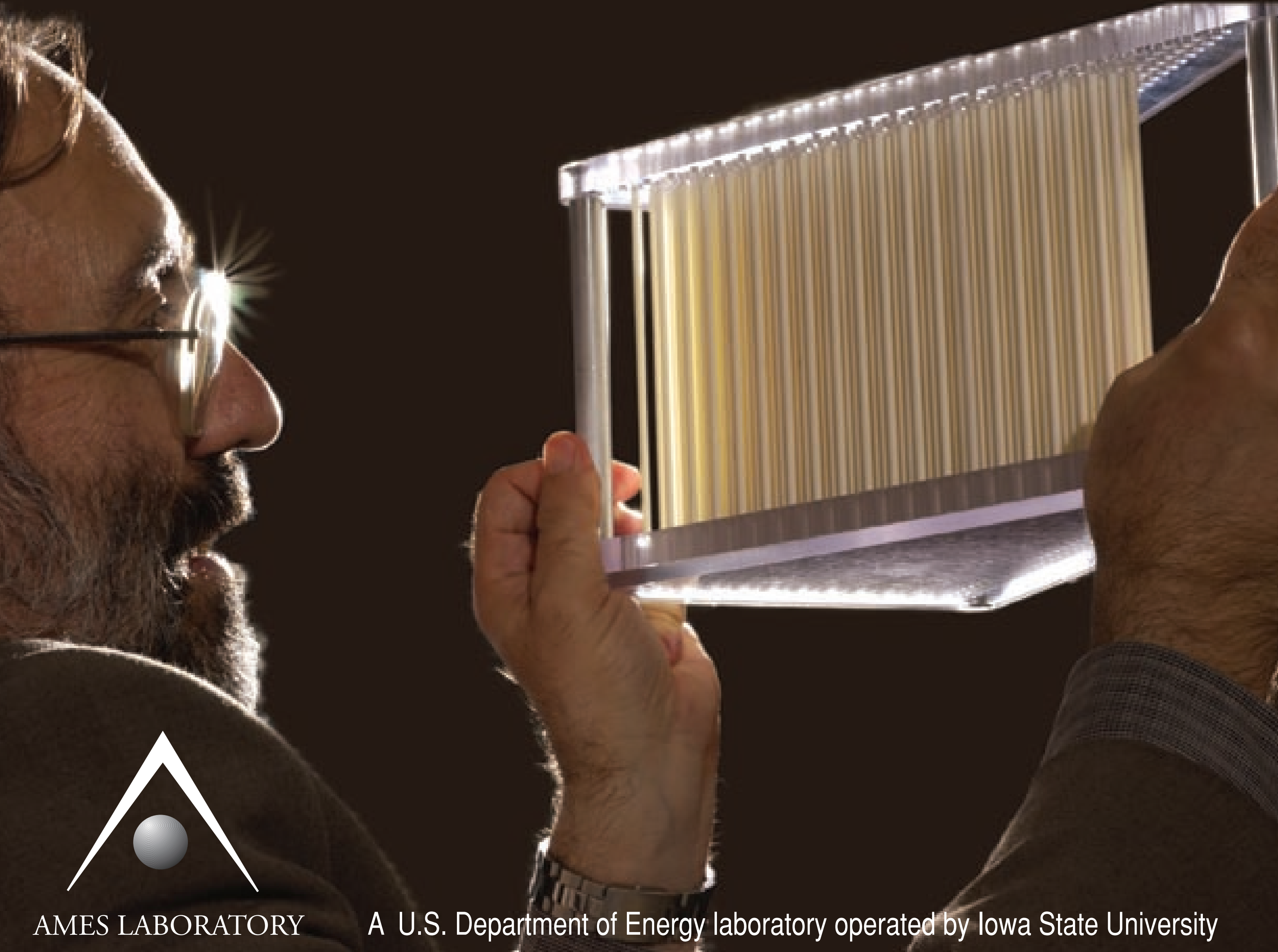
Inquiry 2004

Science and Technology at the Ames Laboratory

Positive attraction of negative refraction
Better catalysts for biodiesel fuel
Adding to the quasicrystal's allure



AMES LABORATORY

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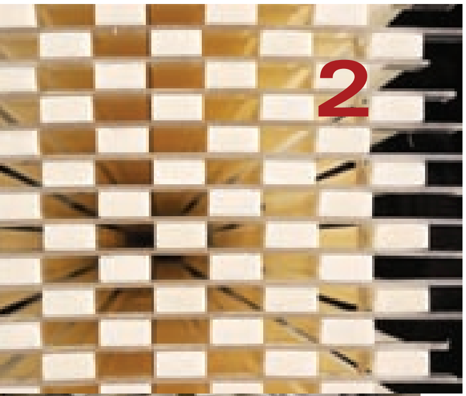

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(front cover) This wedge-shaped photonic crystal being studied by Ames Laboratory senior physicist Costas Soukoulis was designed and constructed as part of a basic research effort to demonstrate negative refraction and superlensing in the microwave region of the electromagnetic spectrum. (see story page 2)

(back cover) Glassware hung up to dry make for unusual laboratory artwork.

from the Director

Welcome to the 2004 issue of *Inquiry* magazine. You've caught me upon returning from a trip to Mexico, combining a chemistry conference and scuba diving. Thus, my guayabera, traditional Mexican attire that has the delightful characteristic of not allowing the use of neckties!

2004 has been a year of rich scientific discovery at the Ames Laboratory, as is evidenced by the variety of stories in this year's *Inquiry*. From groundbreaking research in negative refraction in photonic crystals to a better understanding of the nanoscale surfaces of quasicrystals to developing heterogeneous catalysts for the production of biodiesel fuel, the Ames Laboratory continues to perform cutting-edge research that benefits the Department of Energy and American taxpayers.

In this issue of *Inquiry*, I invite you to read how physicist Costas Soukoulis has confirmed negative refraction in photonic crystals by building and testing a device that when hit by a beam of electromagnetic waves exhibits this formerly impossible phenomenon. The research could lead to the creation of a "superlens" that would provide superior imaging capabilities for a host of medical, environmental and communications technologies.

Also in this issue, you can read how materials chemist Pat Thiel is using scanning tunneling microscopy to examine atomic-scale surface growth of quasicrystals in an effort to better understand how and why these crystalline materials form. The results of her research effort may lead to the creation of new nanoscale technologies.

There's an old saying, "America runs by truck." But this won't be true when we deplete our planet's stock of oil, so Victor Lin is partnering with an Iowa cooperative to develop biodiesel fuel from soybeans. Lin's research involves the development of heterogeneous catalysts that are not only environmentally friendly but could also help lessen the cost to produce biodiesel fuel, creating an even larger market for Iowa farmers' soybean crops.

These stories represent just a smattering of the research you can read about in this issue of *Inquiry*. I hope you enjoy all the articles.

Adios,

Tom Barton

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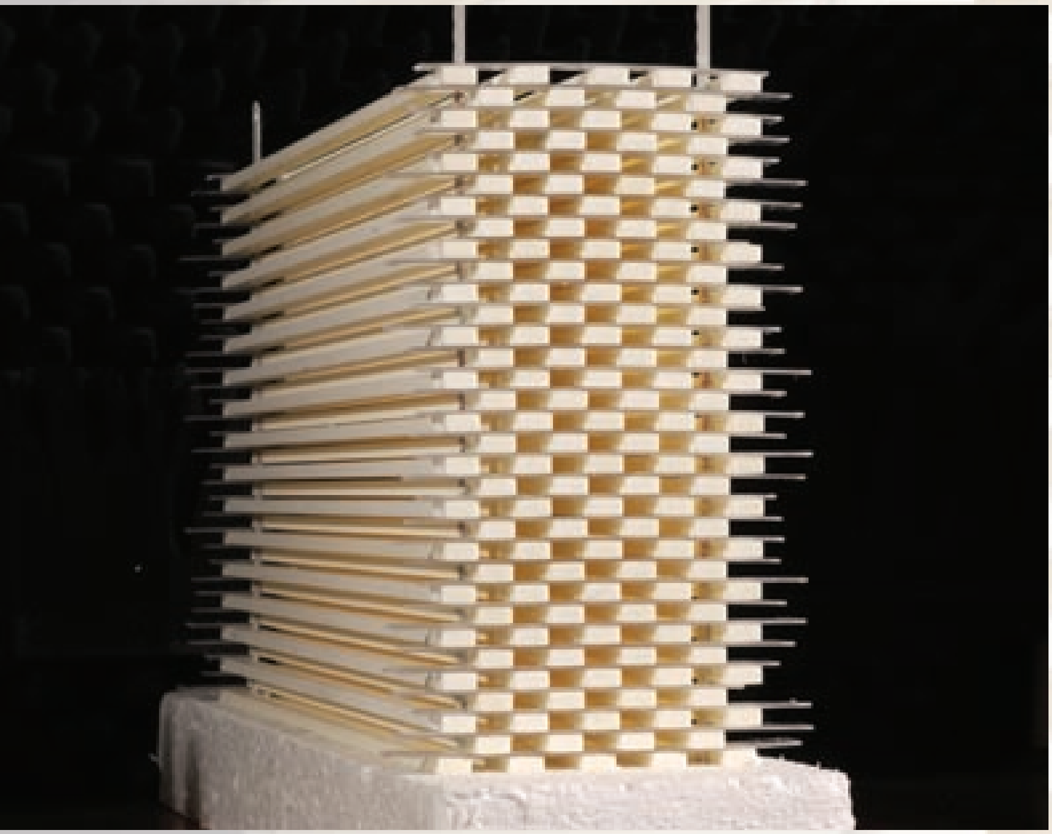
Accentuate the Negative

Physicists are latching on to the positive property of negative refraction

by Saren Johnston



This photonic crystal has a negative index of refraction equal to -1, providing excellent subwavelength resolution. A negative index of refraction equal to -1 is needed to achieve a perfect image.

It doesn't happen naturally, but with the right kind of man-made materials, light can be made to bend, or refract, with a negative angle. When light enters these specially engineered materials, called metamaterials, it takes a sharp turn to the left – a negative turn – bending in the opposite direction to that seen in natural materials. Scientists frequently refer to these unique, synthetic materials as left-handed materials.

Metamaterials and the backward-bending light they allow are drawing considerable attention from physicists because of their range of potential applications. Costas Soukoulis, an Ames Laboratory senior physicist investigating and designing such materials, says left-handed materials may one day lead to the development of a type of flat superlens that operates in the visible spectrum. Such a lens would offer superior resolution over conventional technology, capturing detail much smaller than one wavelength of light to vastly improve imaging for biomedical and materials applications.

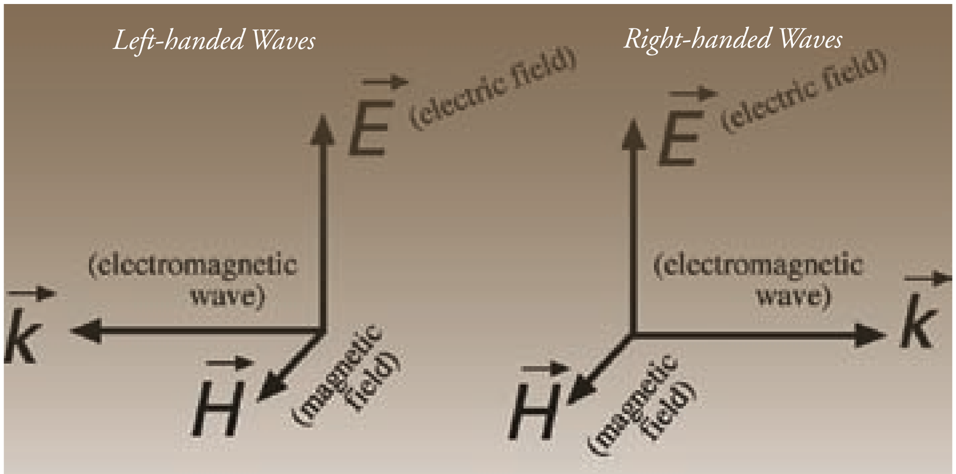
Soukoulis, who is also an Iowa State University physics professor, adds that another unique property of left-handed materials is that they may be fabricated to have zero reflectance for all the incident angles (those which are hit by the incoming electromagnetic waves). It would be difficult if not impossible to determine the location of an object that does not reflect light, so the implications for the development of many applications (including a stealth plane coated with a metamaterial) are obvious.

Thinking negatively

The development of metamaterials and experiments with negative refraction are recent efforts, having drawn little serious attention before the late 1990s. However, Soukoulis notes that the concept of a material with a negative refractive index was first put forth in 1968 by Soviet physicist Victor Veselago of the Russian Academy of Science in Moscow. Veselago envisioned materials with a negative refractive index within which the electric magnetic field and the propagation vector of the electromagnetic wave would form a left-handed triad of vectors – thus the name, left-handed materials.

Although Veselago predicted that left-handed materials would have some unique capabilities, there were no materials available on which he could test his theories. Thirty years would pass before physicists revisited Veselago's hypothesis and began investigating ways to construct the type of negative-index material he had contemplated decades earlier. But once they did, the race was on to construct the perfect left-handed material.

Mixed reaction to negative refraction



Electric and magnetic fields along with the propagating vector for the electromagnetic wave result in a left-handed triad of vectors (E, H, k) for left-handed materials and a right-handed triad of vectors (E, H, k) for natural.

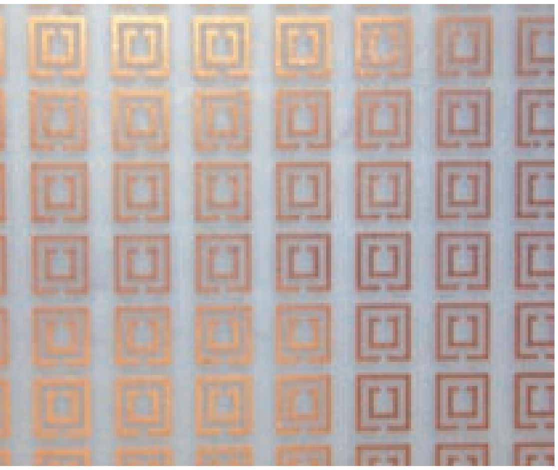
The idea of engineering materials that would refract light negatively stirred up a fair amount of controversy within the scientific community. Soukoulis says many people regarded the idea with skepticism. After all, scientists rely on the principle that every naturally occurring material has a positive refractive index that measures how fast the material transmits light and how the light is bent on entering the material. It's fundamental to the field of optics.

In positive refraction, when light, or electromagnetic radiation, passes at an angle from one material into a different one, such as from air into water, it bends to the right at the point of entry – the boundary between the two materials. Many students first encounter the phenomenon of positive refraction in high school science class when they observe how a pencil placed in a glass of water appears distorted, or bent, to the right at the point where it meets the water's surface.

Negative refraction reverses this well-established configuration and so met with opposition from scientists who believed (and some still do) that it wasn't possible to engineer a true left-handed material. Such a material would have to include a simultaneously negative response to both electric field and magnetic field.

Those questioning the existence of negative refraction say it goes against the

Costas Soukoulis examines one of the photonic crystals that was constructed to observe negative refraction and superlensing in the microwave region of the electromagnetic spectrum.



This metamaterial exhibits the properties required for negative refraction: negative electric permittivity, negative permeability and negative index of refraction.

laws of physics by violating the limit for the speed of light. However, in the midst of the debate surrounding its existence, proponents of negative refraction and Veselago's original thoughts on the subject continue to accumulate more and more proof of its existence.

Negative numbers grow

In the late 1990s, other "negative thinkers" became intrigued with Veselago's ideas on negative refraction. John Pendry of Imperial College in London determined that although negative index materials don't exist in nature, it might be possible to design and construct such materials. Pendry and members of his research group were able to create a synthetic material that showed a negative response to electric field. They quickly followed up on that success by building a second synthetic material that showed a negative response to magnetic field. That left the challenge of combining those properties to create the first metamaterial.

Soukoulis' colleague, David R. Smith of the University of California at San Diego, met the challenge. Smith and his research team were the first to construct and test a material that exhibited a negative response to both electric field and magnetic field in the microwave region of the electromagnetic spectrum. Their metamaterial consisted of small copper loops and wires and showed that microwaves passing through the material were negatively refracted.

Moving down the spectrum

Researchers are just beginning to explore applications for negative refraction at microwave frequencies – and there are many. But even as that work gets underway, some physicists are looking down the electromagnetic spectrum and focusing their attention on visible light. Soukoulis and members of his research team are leaders in that effort. He emphasizes that a material with a negative refractive index for visible light would bring about a remarkable transformation in science and technology.

Unlike natural materials, metamaterials can focus light without the need for curved surfaces. Soukoulis says this characteristic would allow a flat piece of a metamaterial for visible light to serve as a superlens – one capable of focusing electromagnetic radiation to atomic scale length. Potential applications for such a lens include superior imaging for medical and biomedical diagnostics, monitoring air quality, detecting dangerous substances and making it possible to etch ever-smaller electronic devices for cellular and optical communications.

The negative promise of photonic crystals

With the success of constructing metamaterials for microwave frequencies and the desire to create a technology-altering superlens has come an inspired effort by physicists to develop a negative refractive index material for visible light. Working toward that goal, Soukoulis and his research team have been investigating photonic-bandgap crystals, man-made materials that can transmit wavelengths of light up and down the electromagnetic spectrum and so have alternating regions of different refractive indices. The materials are like old friends to Soukoulis, who collaborated with Ames Laboratory researchers Kai-Ming Ho and Che-Ting Chan in 1990 to theoretically demonstrate the existence of the first PBG crystal.

Working with his colleagues at Ames Laboratory and at the FORTH research center in Greece, Soukoulis has done the calculations and developed the first computer simulations that show negative refraction in a two-dimensional, left-handed photonic crystal. Photonic crystals are periodic structures made from dielectric materials – materials that are electrical insulators or in which an electric field can be perpetuated with a minimum loss in power.

The photonic crystal metamaterial Soukoulis and his collaborator, Ekmel Ozbay, at Bilkent University in Ankara, Turkey, designed and tested consists of a square array of alumina rods at which the researchers aimed a beam of microwaves to demonstrate negative refraction and superlensing in the microwave region of the electromagnetic spectrum.

In addition to showing that the incoming beam is negatively refracted, the simulations revealed another significant piece of information. Refraction does not occur immediately. The incoming electromagnetic wave is temporarily delayed and trapped at the boundary between the air and the negative refractive index photonic crystal before it eventually moves in a negative direction.

Soukoulis and his colleagues maintain that the outer rays in the delayed beam give the impression of traveling faster than the speed of light because of this trapping mechanism. Pendry, who performed much of the early research on negative index materials, notes that the calculations and simulations done by Soukoulis' team are "important confirmation that the speed of light is not violated by negative refraction."

Soukoulis says, "The negative refraction effect we've demonstrated depends only on the refractive index of the dielectric material making up the photonic crystal and the geometric factors of two-dimensional photonic crystals. Therefore, this effect can also be observed at optical wavelengths by using transparent semiconductors to obtain similar refractive indices."

Soukoulis' work moves physicists one step closer to constructing materials that exhibit negative refraction at optical wavelengths and realizing the much-sought-after superlens. But, as he says, there is still much to be done. "We want to know more about what happens when electromagnetic waves are directed at a negative index photonic crystal – what causes the delay in the instant before the wave is refracted," he says.

Soukoulis will also continue to work on new designs for 2-D and 3-D negative-refractive-index photonic crystals, and part of that effort will be to resolve the energy losses that become larger and larger with the move to higher frequencies in the electromagnetic spectrum. "Discovering the origin of these losses – that's the theoretical challenge," he says.

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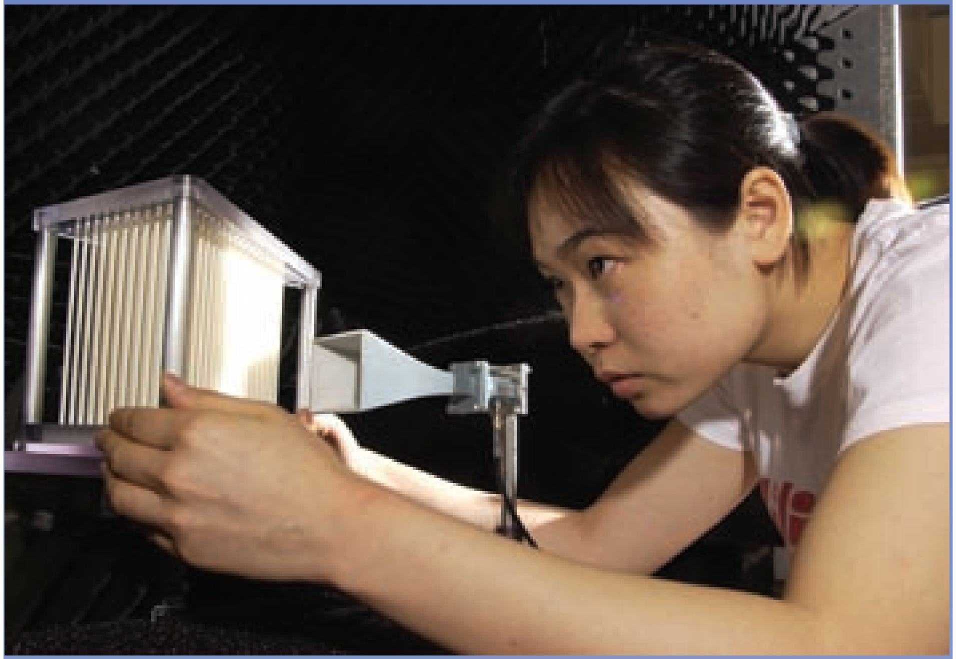
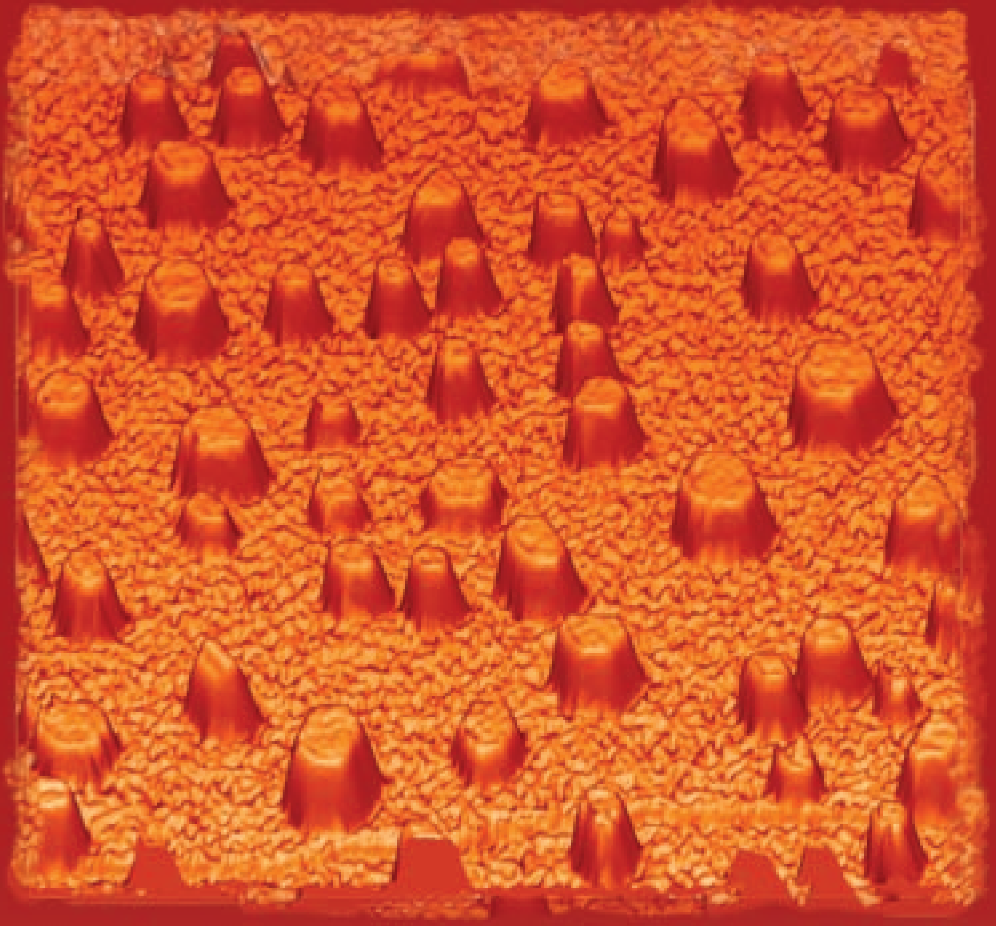


Lei Zhang adjusts a photonic crystal for angle and transmission measurements.

Based on the calculations and simulations done by Soukoulis, experimentalists working on the left-handed materials team are constructing metamaterials and photonic crystals to observe negative refraction. Lei Zhang, an Ames Laboratory graduate assistant working with Soukoulis, carries out many of these experiments under the supervision of Gary Tuttle, an Ames Laboratory associate working at ISU's Microelectronics Research Center. The MRC is a member center of the university's Institute for Physical Research and Technology.

Zhang's experiments with metallic structures built to conform to Soukoulis' simulations support his theoretical results for the microwave region of the electromagnetic spectrum. The metamaterials exhibit the properties associated with negative refraction – negative electric permittivity, negative permeability and negative index of refraction – the combination of which can exist only in synthetic devices.

Zhang's photonic crystal experiments confirm what Soukoulis predicted: negative refraction and superlensing can be observed in photonic crystals in the microwave region. The next step will be to adapt the technology to other regions of the electromagnetic spectrum, with the ultimate goal of reaching the visual region. However, achieving that goal will require the expertise to fabricate the photonic structures at extremely small length scales. Zhang suspects that objective may be a distant one. For now, she says she would be thrilled to create a successful left-handed material closer to the infrared region of the electromagnetic spectrum.



“Stepping” up to Nanoscience

Unusual growth mode leads to more control over atomic-scale structures

by Saren Johnston

The scanning tunneling microscopy, or STM, image above clearly reveals the uniform height and self-organized growth of the PbSi(111) islands studied by Michael Tringides and members of his research group. The majority of the islands are seven layers high.

Advertisers tout them, consumers clamor for them, and manufacturers scramble to meet consumer demand. What causes all this hoopla?

It’s the need or desire, or both, to have the latest-and-greatest, most technologically advanced version of just about anything.

However, the most up-to-date version of a product debuts only after substantial groundwork has been laid. In reality, we owe the availability of new and improved technologies that make our lives easier to a lot of hard work at the research bench. That’s where fundamental science takes place, where researchers study materials and their properties with the goal of developing new materials with better properties.

Everything we see, use or produce – from cookware to computer chips – is made from materials, which are, in turn, made up of atoms. How the atoms are arranged in a material determines the kind of properties exhibited by that material and ultimately by the products made from it.

At Ames Laboratory, senior physicist Michael C. Tringides is involved in a basic research effort to broaden the knowledge base about materials and their properties. He and members of his research group, associate scientist Myron Hupalo and graduate students Vincent Yeh and Michael Yakes, focus their efforts on the microscopic processes that control the growth of custom-made materials.

"Control is the name of the game," says Tringides, talking about the importance of growing atomic structures in uniform sizes and with highly ordered geometries for potential applications that include sensors, switches, lasing materials and semiconductors that allow computer chips to run faster.

Exciting as the potential is for the development of these nanotechnologies (artificially fabricated structures in the nanometer range of 0.1-100 nm) and other microminiature equipment, Tringides is acutely aware of the long hours of fundamental research required to bring them about. The work he and his colleagues pursue may prove critical in the further miniaturization of silicon-based electronic devices, a major undertaking in light of the silicon industry's huge role in technological innovation and production.

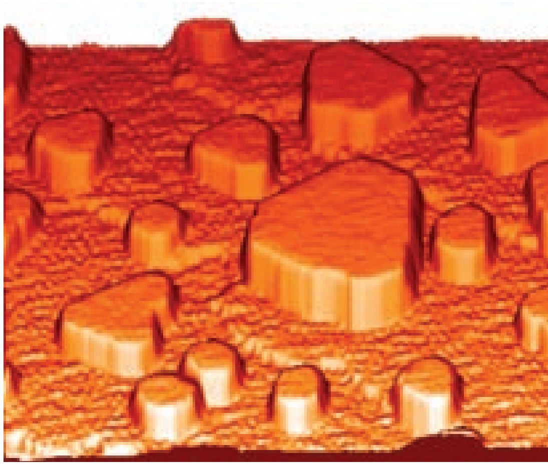
Michael Tringides and his research group are seeking what he says is the "Holy Grail" in nanotechnology – gaining control of layer thickness and atomic uniformity of thin films and nanostructures. (clockwise, from lower left: Tringides, Vincent Yeh, Michael Yakes and Myron Hupalo)

Manipulating miniatures

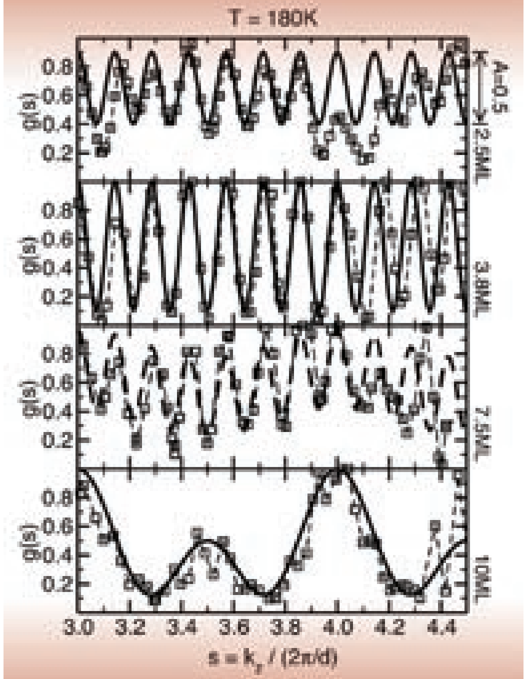
Tringides explains that vital to the success of these miniaturization efforts is the ability to achieve exact control of layer thickness and atomic uniformity of thin films and nanostructures – what he refers to as "the 'Holy Grail' in nanotechnology, the next major industrial revolution."

Noting the great demand for these materials within the silicon industry, Tringides says, "It's essential that these structures are grown in a robust and reproducible way, with easy size selection. Contrary to conventional wisdom, we've discovered that an intriguing type of self-organization is possible with lead (Pb) deposited on silicon (Si) if the growth is carried out at low temperature – around 185 Kelvin, or minus 126 degrees Fahrenheit." He adds that in all other systems studied so far, the deposited metal atoms stack up in islands of very different height variation. But for Pb grown on Si (oriented along the (111) crystal axis), he says the atoms seem to be "intelligent" and make only one height choice.

"The selected height of these nanostructures is related to their electronic structure," Tringides continues. He explains that keeping electrons confined in small metal islands requires them to occupy sharp energy levels as dictated by the laws of quantum mechanics. This confinement implies that the total energy of the electrons depends strongly on the nanostructure's size or shape. "This is called Quantum Size Effects, or QSE," says Tringides, "and a consequence of this relationship is that certain film thicknesses are more stable than others."



Tringides is able to grow Pb islands of five layers by using a different type of silicon surface as the substrate.



Electron diffraction "fringes" (similar to the ones formed when light scatters from a very thin air wedge, but of much larger size) can be used to deduce that practically all islands are seven layers high for lead coverages between 2.5 ML, or monolayers, and 7.5 ML.

Charting new islands

Tringides and his research group were the first to observe and monitor the highly unusual formation of uniform-height Pb/Si islands. They observed the 7-step (or 7-layer), steep-edged, flat-top islands using two complementary techniques. Quantitative electron diffraction, used by Yeh and Yakes, samples the island height uniformity by reflecting electron waves from the surface. Scanning tunneling microscopy, or STM, allows scientists to see the structure of the islands with atomic resolution. STM, used primarily by Hupalo, images the islands and gives the island size and shape directly, without further data analysis. "As a result of our investigations, we have shown that not only can QSE be observed in small objects, but QSE can dictate the island uniformity and height," says Hupalo.

The scientists were amazed to see this uncommon growth mode of the 7-step Pb islands, which clearly shows that the deposited atoms seem able to "climb" and select preferred, final positions. "No one was expecting to see the uniform-height, self-organized growth," says Tringides. "We couldn't believe how quickly the islands formed following deposition. Nature, itself, was doing the work for us!"

Taking control

Tringides explains that although QSE is the driving force for height uniformity, one still needs to find the right temperature and surface coverage conditions for the islands to form. These variables make it difficult to predict when the self-organized growth is possible and explain why it has never been seen before.

"It's necessary to study the growth as a function of the different growth parameters, such as temperature and deposition rate, to discover when such self-organized nanostructures form," says Tringides. By varying these parameters in the Pb/Si(111) system, he and his co-workers found that only odd island heights, i.e. 5, 7, and 9 layers, are possible. Using these growth parameters, they developed a kinetic phase diagram that serves as a guide to select the desired island height.

But Tringides warns that island height uniformity exists only at sufficiently low temperature. At higher temperature, the islands evolve into multiheight mounds, limiting their potential for room-temperature applications. Working to resolve the problem, Tringides and members of his research group have discovered that they can "manipulate the growth" by adsorbing oxygen, which restricts the upward motion of the Pb atoms, allowing the islands to maintain the same height at higher temperatures. This process extends their potential for technological applications. "At the same time, it raises important theoretical questions about how the potential energy surface of the Pb islands is modified by oxygen adsorption," Tringides says.

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"Powering Up"

by Saren Johnston

IBM grant will increase computer power for Ames Laboratory and ISU

Brett Bode, associate scientist in the Ames Laboratory's Scalable Computing Lab, examines one of the three IBM Power 4 workstations that came to Ames Laboratory and Iowa State University through a Shared University Research grant. Each workstation contains eight central processing units for a total of 24 CPUs that will greatly enhance the SCL's parallel computing power.

Massively parallel power just got a boost at Ames Laboratory and Iowa State University with the awarding of an IBM Shared University Research Grant to Mark Gordon. This is the third SUR grant awarded to Gordon, program director of Applied Mathematics and Computational Sciences and an Iowa State University distinguished professor of chemistry. The grant's primary focus is life sciences research.

"Very few SURs were approved for funding – ours and one or two others – so we were very high priority," says Gordon. "Jamie Coffin, my contact at IBM and their vice president of Health Care and Life Sciences Industry, was very instrumental in our selection," he adds.

The SUR grant came through the ISU Foundation to Gordon's chemistry research group in the form of three IBM Power 4 computer workstations. The workstations are valued at approximately $434,000 according to Amy Brockhorn, IBM client executive for Iowa State.

IBM certified pSeries specialist Julie Cray says the three Power 4 workstations, together, contain 24 central processing units, 96 gigabytes of memory, 876 gigabytes of disk space, and 111,870 megaflops of operating power – all of which will substantially increase parallel computing power in Ames Laboratory's Scalable Computing Lab. Computational scientists in the SCL will configure the workstations into a "cluster" to create a 24-node parallel computer.

An identical SUR grant was also awarded to Ken Jordan, a colleague of Gordon's at the University of Pittsburgh. "This is intended to be the first stage in what IBM calls a strategic partnership between Iowa State and Pittsburgh," says Gordon. "A potential aspect of the partnership is a joint postdoctoral position with IBM. That means IBM might fund half of a postdoc position, and I would fund the other half." Gordon says that individual would spend most of the time in Ames, but part of the time doing life-science-related research for IBM at the Maui High Performance Computing Center in Hawaii.

"The Maui Center is mostly funded by the Department of Energy," says Gordon. "It's an IBM shop – all of their computers are IBMs."

According to Gordon, the initial target of the life sciences research will be to learn more about water. "We're developing models that will provide accurate calculations on water molecules, from very small numbers of water molecules to very large numbers," he says. The work will make it possible to simulate both the molecular properties and the macroscopic properties of water molecules.

"All of the biological processes in living things occur in water, so the first step in really being able to simulate those processes is to do very good calculations on water," explains Gordon. "The next step is to look at the processes that are occurring in the water."

Pittsburgh's Jordan, Gordon's SUR grant partner, is also very interested in water clusters. "He uses the models created by other researchers and develops simulation programs," says Gordon. "It's actually a very nice fit because we'll do all the models that he'll use. The partnership will allow for a lot of good interactions."

CREATING POLYMERS THAT ACT LIKE PROTEINS

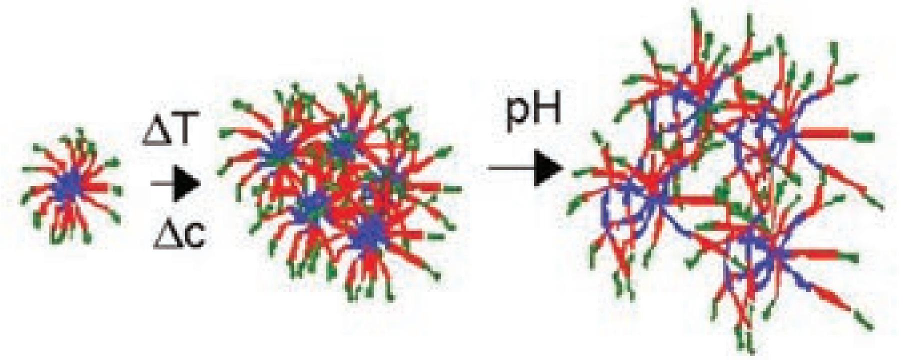
by Kerry Gibson

Ames Laboratory researchers are studying self-assembling polymers

Materials chemist Surya Mallapragada looks at self-assembling block polymers through a cryotransmission microscope.

Even the simplest organisms contain “magical” substances, such as proteins, lipids, and DNA, that react to chemical and environmental cues to perform a variety of tasks from controlling chemical balances to regulating growth and cell reproduction.

Researchers at Ames Laboratory are studying a group of bioinspired, self-assembling polymers to understand how they are able to form and react to stimuli similar to the way proteins, lipids and DNA react in nature. Unlocking how these soluble block polymers are able to self-assemble could potentially lead to a variety of uses, such as controlled release systems for sustained and modulated delivery of drugs or gene therapies.



This schematic shows how clusters, or micelles, of polymer strings group together as the temperature rises (center) and then respond to changes in pH (right). Each string is comprised of five blocks – one hydrophobic block (blue), two hydrophilic blocks (red) and two cationic blocks (green).

Pentablock polymers

Ames Laboratory materials chemist Surya Mallapragada and her research team are focusing on pentablock polymers – polymers that form in strings of five chains. Each string is comprised of two cationic (positively charged) blocks, two hydrophilic (water loving) blocks, and one hydrophobic block. Because the hydrophobic block tries to avoid water, it forms the center of the string, with the hydrophilic next and the cationic blocks on the outside. In solution, these strings form in small clusters called micelles, again with the hydrophobic blocks at the center.

"The interesting thing about these polymers is that they respond to changes in temperature and pH," says Mallapragada, who is also an Iowa State University associate professor of chemical engineering. "As the temperature goes up, the micelles cluster together more, forming a polymer gel. A similar reaction takes place as pH rises – the hydrophobicity of the cationic blocks increases, which also helps in gel formation."

Temp and pH sensitive

As temperature and/or pH drops, the process reverses itself, and the gels dissolve back into micelles and polymer strands. Using cryotransmission electron microscopy, Mallapragada's group is working to understand just how these micelles look and how fast the polymers respond to changes in temperature and pH.

"Samples are plunged into liquid ethane, which freezes them so quickly that ice doesn't form and disrupt the crystal structure," she says. "We're able to then view the gel formation at various stages (temperature and pH) under very controlled conditions." She adds that this work will be complemented by conducting X-ray scattering studies at the Advanced Photon Source facility at the Department of Energy's Argonne National Laboratory.

The structure appears to be the key in how the polymers react to stimuli similar to the way biomolecules react in nature. These substances carry out a wide variety of tasks, responding to subtle changes in body chemistry regulating those changes. The problem in working with proteins and similar biomolecules, according to Mallapragada, is that it is difficult to isolate the materials without damaging them.

"Biomolecules often exist in extremely small quantities," she says, "and are not very robust. In separating them from a source, they become denatured, or damaged. The polymers we are studying are much more stable, readily available and therefore easier to study."

Delivery potential

Because they are easier to work with, the polymers could potentially be modified and used as a way to deliver drugs or gene therapies. For example, incorporating the glucose-oxidase enzyme in the polymer would make it sensitive to changes in glucose levels in the body. Soluble at room temperature, the polymer could be injected under the skin where it would form in a gel due to the higher temperature of the body. When the gluconic acid level falls, the resulting drop in pH would cause the polymer to swell and release insulin.

The injectable gels would be much less invasive than surgically implanting automatic insulin delivery systems, and the gels would dissolve on their own after about a week.

For potential gene therapies, the positively charged (cationic blocks) polymers can complex with DNA (negatively charged). The polymers could be used to deliver so-called suicide genes and chemotherapy drugs directly and selectively to tumors, since normal cells would be less likely to react with the polymer and express the incorporated gene.

A preliminary in vivo study in rats, funded by an ISU Bailey Career Development Grant, is now underway in conjunction with the John Stoddard Cancer Center at Iowa Methodist Medical Center in Des Moines.

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Research funded by:

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Materials Chemistry Division

MODEL BEHAVIOR *for* Random Materials

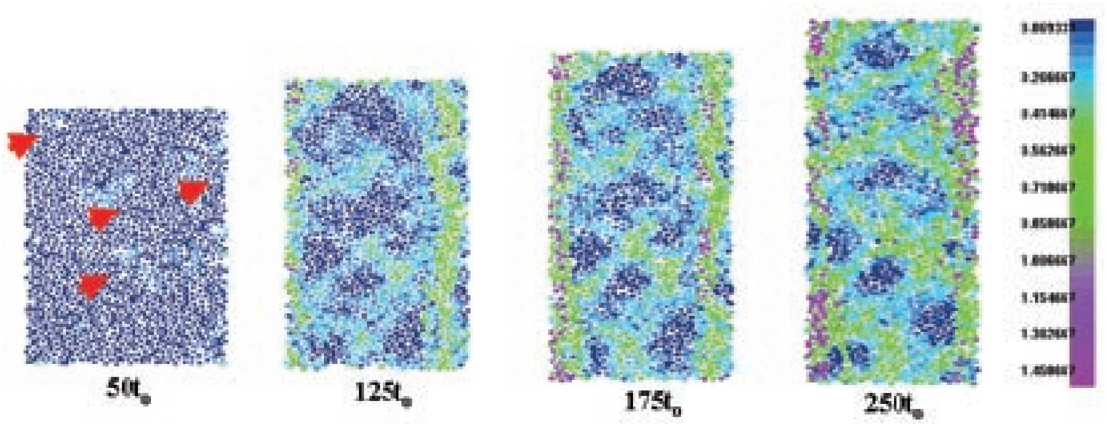
by Kerry Gibson

Metallurgist Bulent Biner sits next to the powerful computer cluster used to generate his molecular dynamics simulations of the deformation behavior of metallic glasses.

Since the 1960s, scientists have marveled over amorphous metal alloys, materials also known as metallic glass, for their unique physical, and sometimes electrical and magnetic, properties. Now researchers at Ames Laboratory are closer to answering how these materials are able to take on certain high-strength and elastic properties that stem from their "glassy" origins.

Metallic glass can be formed in various ways, but the most common is by quenching a molten metal alloy so quickly that its normal crystalline structure doesn't have a chance to form. Instead, the atoms are randomly scattered along with empty regions, so-called free volume. This lack of crystalline structure gives metallic glasses high-strength, elastic properties that make them more rigid than ordinary metals/alloys. These good mechanical properties are accompanied by very low ductility at room temperature. Yet by heating metallic glasses to a few hundred degrees Centigrade – but still below their melting points – they can be formed into very complex shapes.

It's these deformation behaviors that Ames Lab metallurgist Bulent Biner is seeking to explain.



This graphic representation shows the evolution of microstructure with time during deformation under constant stress. Atoms were colored depending on the strain they accumulated, and arrows indicate the location of the free volumes as observed during the MD simulations.

Flipping a switch?

"These materials seem to have a switch mechanism near their transition temperature," says Biner, who is developing molecular dynamics simulations to try to explain these peculiar materials. "At lower temperatures, when stress is applied, the deformation that takes place is inhomogeneous — small clusters of randomly packed atoms appear to work in concert to form so-called shear transformation zones.

"These zones localize displacements in surrounding regions that trigger the formation of highly localized shear bands during the deformation," Biner continues. "In other words, the deformation spreads out from these zones as we see in granular materials like sand."

As temperatures approach a metallic glass' transition temperature, however, the deformation is no longer localized and becomes uniform. Individual atomic jumps are the basic step in the mechanism of this homogenous deformation. In order for individual atomic jumping events to take place, there should be enough free volume (open space) in the immediate neighborhood to accommodate the volume of the jumping atom.

Furthermore, the applied stresses may cause additional creation of free volume by squeezing the atoms into a smaller available free volume by displacing the surrounding neighboring atoms. However, this extra-created free volume is quickly distributed among the neighboring atoms by local rearrangement, a process called annihilation.

Excess Free Volume

The fascinating thing Biner has observed in computer simulations is that as the stress on the materials is increased, the material reaches a point where it can't deform fast enough to annihilate the free volume created, which helps explain how the material goes from elastic to plastic to its breaking point with the accelerated rate of deformation.

"The main switch mechanism seems to be the free volume," he says. "What happens in the low stress region is you are creating free volume but it's annihilated away – there's no excess. In a way, the deformation keeps up. When you move to the higher stress region, excess free volume is created and it becomes like a sponge with lots of voids, and then it finally breaks."

To model this behavior, Biner uses a two-dimensional binary system – "to keep things simple" – with a ratio of .81 between the two atom types. However, even with a "simple" system, the computations necessary to generate the simulations require a significant amount of computer power and execution times of many days, even when carried out on the powerful clusters of computers in Iowa State University's physics and astronomy department. The model system was subjected to constant stress levels, ranging from 0.1 to 0.45 micro-pascals and the axial strain calculated over time. To view computer-generated molecular dynamics simulations of the deformation in progress, go to the Materials and Engineering Physics Web site at http://www.metcer.ameslab.gov/research/amorphous/aahighlights.html.

These values were then used to generate additional data, all of which closely matches the experimental data generated by Ames Laboratory scientists Dan Sordelet and Matt Kramer in their studies of these extraordinary materials. The apparent match of theoretical and experimental brings the researchers closer to understanding these unqiue materials, and that's what makes the effort worthwhile for Biner.

"In the long run, that's what we're trying to understand – how the free volume evolves by the atomic arrangements and hopefully allows us to make a better system," Biner says.

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Research funded by:

DOE Office of Basic Energy Sciences,
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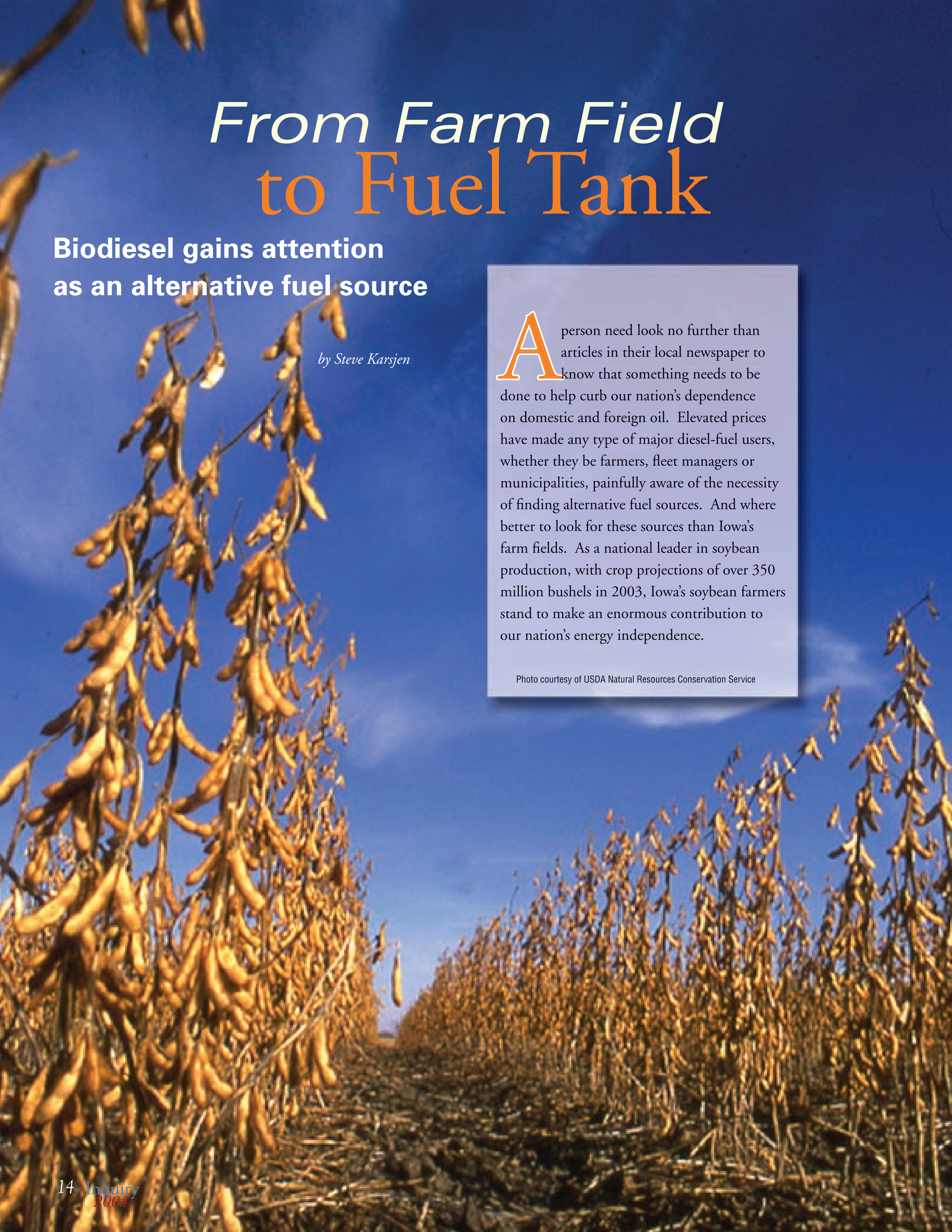
From Farm Field to Fuel Tank

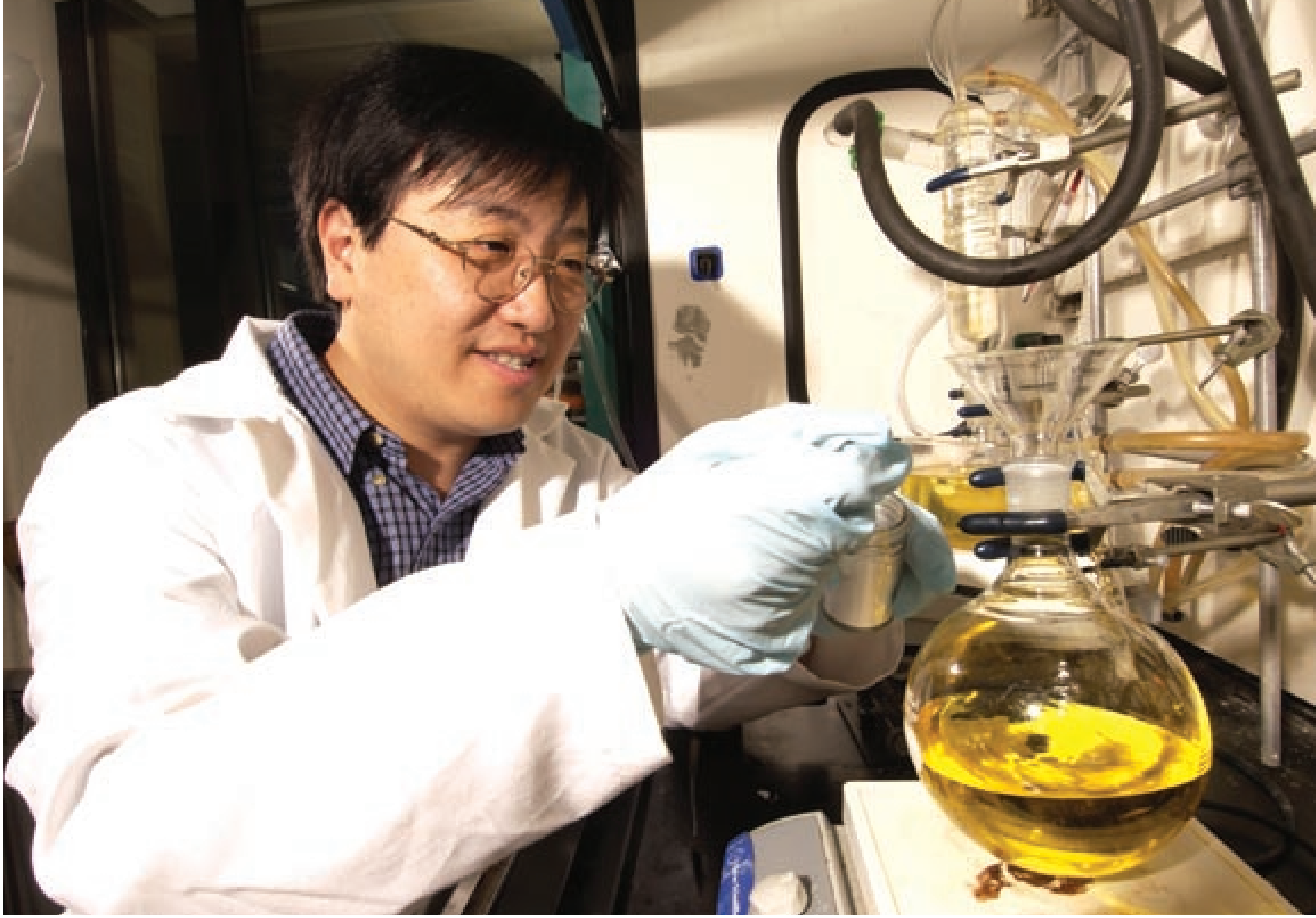
Biodiesel gains attention as an alternative fuel source

by Steve Karsjen



A person need look no further than articles in their local newspaper to know that something needs to be done to help curb our nation's dependence on domestic and foreign oil. Elevated prices have made any type of major diesel-fuel users, whether they be farmers, fleet managers or municipalities, painfully aware of the necessity of finding alternative fuel sources. And where better to look for these sources than Iowa's farm fields. As a national leader in soybean production, with crop projections of over 350 million bushels in 2003, Iowa's soybean farmers stand to make an enormous contribution to our nation's energy independence.

Photo courtesy of USDA Natural Resources Conservation Service



Victor Lin adds some heterogeneous catalyst to soybean oil to create biodiesel.

Soydiesel, or biodiesel, is one of the products gaining favor as an alternative fuel because it's clean burning and biodegradable and can be made from a renewable resource, in this case, soybeans. It's also being eyed as a more environmentally friendly industrial solvent that could be used for the removal of graffiti or for cleaning up oil spills. But there are several keys to making soydiesel more attractive as a fuel – some related to the fact that industry is not geared up to produce biodiesel on a large scale. Other more significant issues relate to the costs of producing it and disposing of the wastes created by the production process.

The effort to discover more efficient catalysts got its start with the help of a Science with Practice grant from the Iowa State University Center for Catalysis and the Ames Laboratory Biorenewable Resources Consortium. The successful results of that research led to the awarding of a $1.2 million grant from the U.S. Department of Energy and U.S. Department of Agriculture, which will be used to study new technologies for production of methyl ester, or biodiesel, from soybeans.

"Our new technology has the potential to reduce energy consumption, enhance economic competitiveness and lower the environmental imprint of methyl ester production," says George Kraus, director of the BRC and the CCAT, and an ISU professor of chemistry.

Catalysts are key to converting triglycerides like soybean oil to biodiesel. To create biodiesel from soy oil, scientists perform a chemical reaction whereby they replace the glycerol in the oil with methanol. This process requires the use of a catalyst. Catalysts are used to speed up the rates of chemical reactions without getting used up in those reactions themselves. The current process to convert soy oil into soydiesel relies on the use of homogeneous catalysts. The process, called transesterification, replaces one ester in the soy oil with another to create biodiesel.

But there are problems with using homogeneous catalysts to manufacture soydiesel. In the example just mentioned, sodium methylate is the preferred homogenous catalyst. It mixes with methanol and soybean oil to create biodiesel. Because it is a strong caustic and corrosive base, the remaining sodium methylate in the biodiesel product mixture cannot be reused and must be neutralized with an acid, which adds unwanted expense to the biodiesel production process.

Also in the mix, is an expensive waste-storage problem because homogeneous catalysts are not easily recyclable. In

Victor Lin and graduate students Hung-Ting Chen and Jennifer Nieweg line up behind samples (left to right) of poultry fat, soybean oil and biodiesel.

addition, the time it takes to do all of this is another factor. When combined, these issues make biodiesel production less financially attractive to producers, like West Central Cooperative of Ralston, Iowa. West Central is a large, farmer-owned cooperative in west central Iowa that annually processes approximately 72 million pounds of soy oil into biodiesel. West Central sells this product to distributors nationwide.

"The success of biodiesel all comes down to costs," says Myron Danzer, sales and production manager for West Central. And like any business, West Central wants to keep costs down and profits high. Doing so will require reducing the costs to produce biodiesel and eliminating the waste problem that comes with using homogeneous catalysts in the transesterification process.

The solution to both problems could lie in the development of heterogeneous catalysts. Because heterogeneous catalysts can be easily separated from the product by filtration, using them eliminates the expense of having to add acid to the biodiesel production mix. Also, in contrast to the nonrecyclable homogeneous catalysts, the heterogeneous catalysts can be reused many times, which further lowers the cost of the biodiesel production.

To find someone doing research in the area of heterogeneous catalysts, West Central had to travel only about 60 miles up the road to the Ames Laboratory and Iowa State University. Catalysis is currently a research thrust of the Ames Lab's Biorenewable Resources Consortium and Victor Lin, an Ames Lab chemist and an ISU assistant professor of chemistry. Lin's research is in the production of heterogeneous catalysts. Through the DOE/USDA grant, Lin and West Central are collaborating to scale up production of test heterogeneous catalysts, analyze tests and design equipment to mass produce new catalysts.

The effort to design a more efficient biodiesel conversion process revolves around Lin's work in the area of "mesoporous silica nanocatalysts." These honeycombed particles speed up the conversion process and can be more easily separated and recycled after they've done their job.

"If we can replace the homogeneous catalyst with one that's heterogeneous, it would allow us to isolate the catalyst and also recycle it so we don't have to waste time and effort trying to neutralize the base catalyst with the acid," says Lin.

Free Fatty Acids

Creating biodiesel from soybeans is just one chapter of the story for Ames Laboratory and West Central. The cooperative would like to expand the variety of products it uses as feedstock to produce biodiesel. One of the items at the top of the list of potential "other" materials is corn. Iowa farmers harvested around 1.87 billion bushels of corn in 2003, so the potential exists for a major market for this product. Other feedstocks also on the list are poultry fat and waste grease. "We want the capability of using what they call multiple feedstock," says Danzer.

Unfortunately, these feedstocks are more expensive to turn into biodiesel than soy oil because they contain a small amount of free fatty acid, or FFA. Some oils oxidize, or become acids if they sit too long. Then they hydrolyze and react with the base, forming a salt that kills the base catalyst before the base can react with the methanol used to create biodiesel.

"So what we're trying to do is create a catalyst that instead of being a base is actually an acid, which will eliminate the free fatty acids before the oils go through the conversion process to produce biodiesel," says Lin. "If companies like West Central can solve this free fatty acid problem, they would be able to really open up their markets," he adds. "For example, there's a 10 cent per pound cost difference between using poultry fat than using soybean oil to create biodiesel."

Two-fold process

At the same time Lin is working on the free fatty acid problem, one of his colleagues, John Verkade, an Ames Laboratory associate scientist and an ISU professor of chemistry, is working to develop a "superbase" catalyst he patented through ISU that would more efficiently conduct the transesterification process, that is converting the triglycerides to biodiesel. "So my participation is to help John design a system to actually turn the homogeneous superbase catalysts into heterogeneous systems so these catalysts can be recycled," says Lin. But going beyond that, Lin says he has developed a new heterogeneous alphacatalyst, containing both an acid and a superbase, which would eliminate the free fatty acids and also do the transesterification.

"What you'd have is a heterogeneous double catalyst," says Verkade, "one that would convert both the FFA and triglyceride to biodiesel."

Lin adds, "Having one catalyst doing two jobs would be like killing two birds with one stone." He notes that this next generation super-efficient catalyst would be useful to industry in many ways. "Efficiency is what they're after, so we would be lowering the costs associated with producing biodiesel as well as making the catalysts recyclable."

As one might imagine, all of this is music to the ears of West Central Cooperative. "Our interaction with Victor Lin has been great," says Danzer. "They get input from us on the practical commercial applications, and we get the detailed science."

Lin says the cooperative is looking beyond just being able to produce biodiesel fuel. "It is also considering selling the overall production design to potential clients," he says. "Let's say, for example, that California wants to build a biodiesel plant. They could come to West Central and purchase an entire design package. That would be good for them and good for us because they would have to buy the catalyst from us."

West Central has actually taken steps to get this process started. It has formed a partnership with another Iowa company to build what Danzer calls "turnkey" plants for other companies.

Lin believes the Ames Laboratory scientists are on the right track to make biodiesel a competitive alternative fuel. "I think we're at a crucial juncture that will require both know-how and government funding," he says.

"Tooling up" the biodiesel production process will require a major change in infrastructure because that infrastructure is currently based on fossil fuels, says Lin. And changing infrastructure always costs money, which he says is where the government comes in. "If some changes are made, we could see the market for biodiesel really open up," Lin concludes.

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Research funded by:

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A worker at the West Central Cooperative processing plant kneels beside a pair of decanters used to separate the lighter methyl esters from the heavier glycerine.

Photo courtesy of West Central Cooperative

Deciphering the Quasicrystal

Starfish and Farey trees add to the quasicrystal's allure

by Kerry Gibson

Ames Laboratory materials chemist Pat Thiel holds a sea-dwelling starfish that exhibits the same five-sided symmetry as a recently discovered phenomenon in which aluminum atoms deposited on a quasicrystalline substrate cluster around site-specific holes in the substrate surface in a star-shaped pattern.

Since their discovery more than 20 years ago, quasicrystals have intrigued scientists with a uniqueness and perfection that defies the conventions of regular crystalline materials. In a similar fashion, an interdisciplinary group of Ames Laboratory researchers is drawing on a unique blend of techniques and talents to lead the effort to decipher how and why these materials form.

First discovered in 1982 at the National Institute for Standards and Technology by researcher Dan Shechtman, quasicrystals are metallic alloys, most of which contain 60 to 70 atomic percent aluminum. These mysterious metallic alloys are somehow able to form into crystals – usually with a five-fold symmetry – in which the atoms are ordered, but without the periodicity common in crystalline materials. Though a direct correlation to the atomic structure has yet to be drawn, quasicrystalline materials are hard, slippery, poor conductors of heat, and resistant to attack by other chemicals. Such properties make them particularly useful for applications requiring resistance to wear, low adhesion or a thermal barrier.

Scratching the surface

Because such properties relate to interactions taking place on the surface of the materials, study of the surface of quasicrystals was a logical starting point. It was also a particularly attractive problem to materials chemist Pat Thiel, who specializes in surface characterization of materials.

"There were some wild speculations about the surface of quasicrystals, but when we started, those hadn't been backed up by experimental data – no one had really taken a look at what was happening on the surface of these materials," says Thiel, who credits Ames Laboratory physicist Alan Goldman for introducing her to the subject and for fostering the Lab's ongoing research efforts in the quasicrystal field.

"It took us a year or so to formulate the specific questions that needed to be asked," she says, "like what is the structure of the clean surface." According to Thiel, who is also an Iowa State University distinguished professor of chemistry, even that seemingly simple question was controversial.

Though lacking a periodic structure, quasicrystals do contain small clusters of atoms. "To create a flat surface would mean cutting through some of the atom clusters, and a segment of the research community believed that you couldn't do this and have a flat surface that was also still quasicrystalline," Thiel says, adding that the notion was dismissed as heresy by some of the more fervent quasicrystal devotees.

Because many quasicrystalline materials are aluminum-rich and because aluminum oxidizes very easily, it was necessary to prepare and study samples in ultrahigh vacuum to look at a "clean," unoxidized surface.

Thiel's group developed a method to clean the surface of quasicrystalline aluminum-copper-iron samples with an ion beam to remove any surface oxidation, followed by heat treatment. Using a number of techniques, including low-energy electron diffraction, her group discovered the surfaces are indeed flat *and* quasicrystalline.

They also found that there are clearly layers, as evidenced by stepped "terraces" on the cleaned sample. Consistent with basic surface science principles, the surfaces of these layers were aluminum-rich and densely packed, and each layer was comprised of two planes of atoms, 0.4 Angstroms (Å) apart. The visible steps were the separation between the favored terminations.

Additional study of these layers showed that there are recurring features, so-called "flowers" of atom clusters. The flowers were comprised of 20 atoms of aluminum, arranged in two rings around one iron atom. By connecting the iron centers of these flowers, a clearly pentagonal, long-range order emerges in an otherwise aperiodic material.

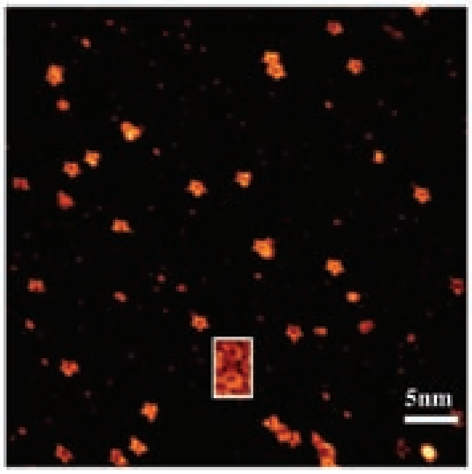
Starfish phenomenon

With this new detailed understanding of the surface, the next step was to look at depositing material back onto a clean quasicrystalline surface to see if it would act like a template, a phenomenon called pseudomorphism. To do this, Thiel turned to thin-film techniques that allow layers only a few atoms thick to be deposited.

"We know that pure silver, for example, doesn't want to form a quasicrystal in bulk," Thiel says, "but this might be a way of forcing it to form a quasicrystal for at least one or two atomic layers. Then we could see if it had unusual properties due to the quasicrystalline structure it was forced to adopt."

Silver and aluminum were chosen because they have low surface energies. In other words, they easily spread out to "wet" the substrate to which they're applied. To deposit these materials, a molecular beam source was used to vaporize pure aluminum, and the gaseous atoms then landed on the clean surface of the substrate.

"These atoms, we believe, are quite mobile," Thiel says. "To our surprise, they seem to find very specific sites on the surface and form in unique arrangements that look like starfish."



This scanning tunneling electron micrograph of the quasicrystalline substrate shows how the atoms of aluminum, deposited using thin-film technology, gather in star-shaped clusters around 2 angstrom-deep holes. This site-specific nucleation and the fact that the "starfish" are uniform in size represents a breakthrough in the understanding of the surface characteristics of quasicrystalline materials.

The "starfish" are comprised of five, or possibly six, atoms of aluminum that gather in a star shape around 2 Å-deep holes in the surface of the materials. At this point, it's not clear if a sixth atom locates in the center hole.

"This is remarkable for a couple of reasons," Thiel adds. "In a normal crystalline material, you have homogeneous nucleation where the deposited atoms diffuse and collide, and randomly form new islands on the substrate. Here, we see site-specific nucleation – the atoms diffuse and cluster at the holes, which are trap sites.

So the surface is dictating the nucleation, and the arrangement of these nanostructure islands is not at all random.

"The other interesting thing is that the atoms are arranged pseudomorphically," Thiel says. "The aluminum atoms arrange in a pentagonal symmetry that they would not want to adopt in the bulk. The starfish are also nearly identical in size, which is another level of control not normally seen. Nature has manufactured something that's remarkably uniform."

Following Fibonacci

Starfish aren't the only remarkable new phenomenon associated with quasicrystals that Ames Lab researchers have discovered. While alloys are known to exhibit quasicrystallinity in two and three dimensions, materials chemists Gordon Miller and Olivier Gourdon appear to have discovered a one-dimensional (linear) quasicrystal in a zinc-palladium alloy. Viewed in a single plane, polyatomic clusters of zinc and palladium atoms form in a repeating motif that appears to approach a limiting case described by the Fibonacci sequence.

The Fibonacci sequence, named for the 13th century mathematician who first described it, is one of those mathematical puzzles that demonstrates order from what initially appear to be random occurrences. In his original treatise, Fibonacci used a scenario in which a pair of rabbits would produce one pair of offspring each month. Given that each successive generation would take one month before reaching maturity and producing yet another pair, Fibonacci asked how many rabbits would be produced in the course of a year.

The solution can be found by what is known as a recursive sequence, in which you simply sum the two preceding terms to find the next one. In the case of the rabbits, one pair is produced during each of the first and second months. The third month, the original pair and the first pair of offspring each produce a pair. Three pairs are produced the fourth month, then five, etc, producing the sequence of numbers 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233 and so on.

"One of the beauties of quasicrystral research, particularly here at Ames Laboratory, is that it is truly interdisciplinary.
— Gordon Miller

In a so-called Farey tree, the "starting" numbers are expressed as fractions. Adding the numerators and denominators of those and subsequent fractions recursively, results in a cascading series of values that become greater in number but closer in value as shown in the diagram on page 21.

The Zn-Pd system Miller and Gourdon are studying seems to follow the same type of recursive sequence as the concentrations of the two components are varied.

"It gives us a possible recipe," Miller says of the combinations suggested on the Farey tree. "We can target certain compositions to see if they indeed give rise to an identifiable unit cell."

Miller's interest in the zinc-palladium alloy stems from a phase diagram of the material. The diagram shows a region of roughly a 70 percent to 80 percent concentration of zinc, that indicated a metastable "gamma brass" state normally associated with quasicrystalline behavior.

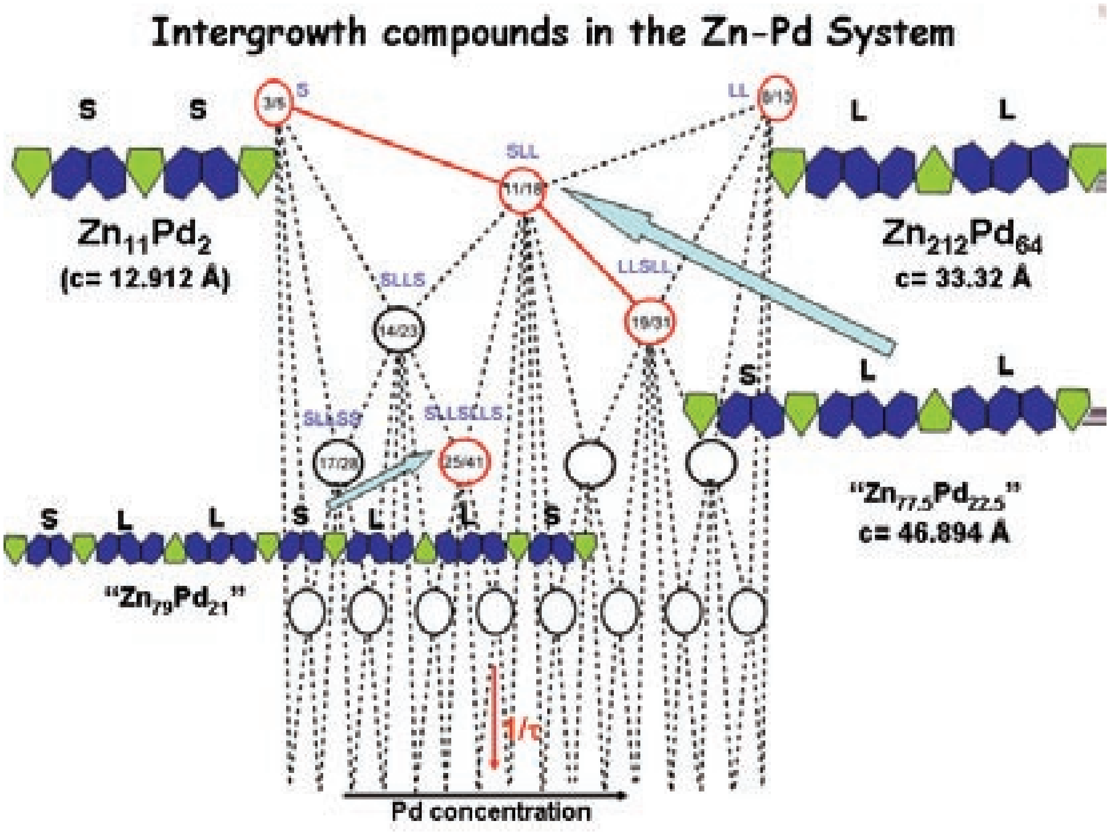
At one side of this phase region, a sample of $Zn_{11}Pd_2$ exhibited a short linear arrangement of zinc and palladium atoms that, through the use of X-ray diffraction, measured 12.912 Å long. At the other side of the phase, a $Zn_{212}Pd_{64}$ composition exhibited a long linear arrangement that measured 33.32 Å.

"We wondered if other compositions would be expressed as combinations of these short and long strings," Miller says. "So far, we've been able to show that compositions for $Zn_{77.5}Pd_{22.5}$ and $Zn_{79}Pd_{21}$ fall as expected (according to the Farey tree model) with longer and longer clusters comprised of a repeating sequence of short and long strings.

"Does this system continue to follow the sequence?" Miller asks rhetorically. "We don't know yet. As the unit cells get longer, the diffraction points displayed get closer and closer together, and given our current measuring instrumentation, there comes a point where we can't differentiate between individual points anymore."

According to Miller, the value of this and similar research is that it leads to new ways of thinking about how materials form, especially as they go from liquid to solid state.

"One of the beauties of quasicrystral research, particularly here at Ames Laboratory," Miller says, "is that it is truly interdisciplinary. The study of metals has traditionally been the realm of physicists, metallurgists and crystallographers, but these materials have gotten chemists involved, and the molecular viewpoint we bring can aid the field in helping interpret what's taking place."



This diagram shows how Miller and Gourdon were able to use a Farey tree model to predict the unit length of different compositions of compounds in a zinc-palladium system. The top two compositions represent the "borders" of the quasicrystalline gamma brass phase and represent short and long one-dimensional atomic clusters. As the tree cascades down, the subsequent compositions are made up of corresponding combinations of short and long clusters.

World-class attraction

One other very key aspect of this group approach is the access Thiel, Miller and others have to large-scale sample quasicrystalline materials to study.

"We're extremely fortunate to have the world's leading experts in growing crystals in Ames Laboratory researchers Tom Lograsso and Paul Canfield," Thiel says. "And their work is made possible by the availability of ultrahigh purity metals produced by the Lab's Materials Preparation Center."

Lograsso, using Bridgeman and other crystal-growth techniques, has produced a variety of quasicrystalline materials, including a 25 cm^3 single crystal of icosahedral cadmium-ytterbium ($Cd_{84}Yb_{16}$). Canfield specializes in flux-growth methods for producing rare-earth magnesium-zinc, single-grain quasicrystals.

At the other end of the sample size-spectrum, senior scientist Dan Sordelet has successfully worked with hot isostatic pressing and sintering techniques to develop quasicrystalline coatings from gas-atomized powders, work that also relies on the MPC for the purest materials available.

As a reflection of this overall strength in quasicrystal research, Ames Laboratory will host the Ninth International Conference on Quasicrystals – ICQ9 – in May 2005.

And Shechtman, the researcher who started it all, will be joining the Ames Laboratory staff periodically over the next several years as a visiting scientist on leave from his permanent position at the Technion in Israel.

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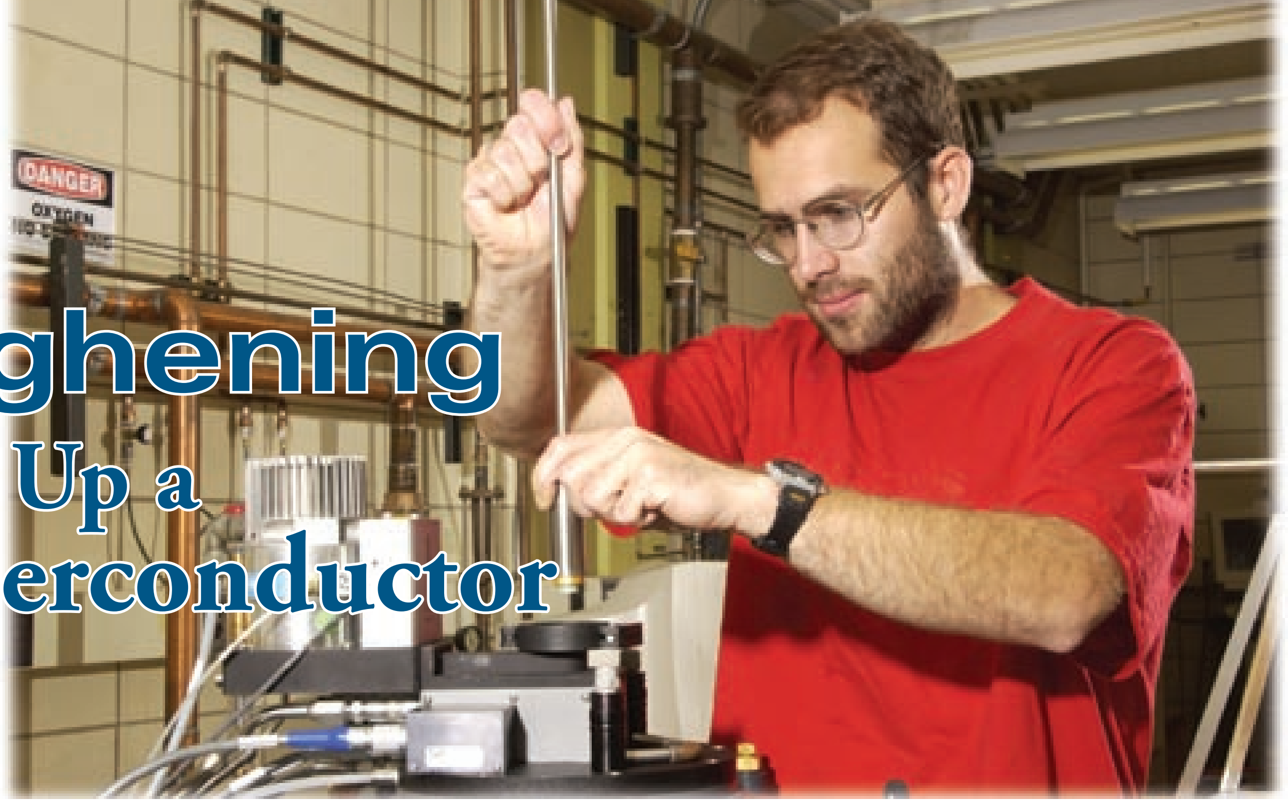
Toughening Up a Superconductor

by Saren Johnston



Derek Wilke inserts a puck holding a carbon-doped MgB_2 wire sample into the quantum-design physical property measurement system. The instrument contains a 14 Tesla superconducting magnet for performing magnetotransport measurements that are used to determine the sample's upper critical magnetic field.

Researchers find a little dab of carbon adds "character" to MgB_2

Carbon is the sixth most abundant element in the universe. It exists all around us in nature, and its applications vary tremendously with its form and properties. We easily associate carbon with such items as pencils, diamonds and steels, but it's also found in plastics, paint pigments, lubricants, clothes and cosmetics. It's present in many foods, for example, asparagus is especially high in carbon. It's found in the sun, stars, and atmospheres of most planets. And we know that all living organisms contain carbon – there would be no life without it. The fact is, the big "C" is such a "popular" element that there are more than 18 million compounds of carbon listed with the Chemical Abstracts Registry, a registry system for all completely identified chemical compounds.

Now, a group of Ames Laboratory physicists have added carbon to a superconducting compound, magnesium diboride, in a basic research effort to enhance the properties of the material. By doping MgB_2 with carbon atoms, they have doubled the magnetic field the material can withstand. The work may one day ease the expense associated with current superconducting materials that generate the intense magnetic fields required for such applications as magnetic resonance imaging for medical diagnostics, high-field magnets for research, and superconducting magnets for particle accelerators. The fundamental research on MgB_2 is part of an experimental effort on superconductivity and correlated systems at Ames Laboratory.

MgB_2 history

Unlike ordinary conductors, such as copper, superconductors conduct electricity perfectly, without energy loss due to heat. But metallic superconductors, most notably triniobium-tin, Nb_3Sn, have always been hampered by the fact that they must be cooled to an extremely low temperature before they become superconducting. That critical temperature, or T_c, rests near absolute zero (0 Kelvin or minus 459 degrees Fahrenheit), thus cooling has always been expensive, requiring large quantities of liquid helium.

However, things warmed up in 2001 when scientists discovered the superconducting properties of magnesium diboride. They were amazed to see that the critical temperature at which MgB_2 becomes superconducting is 39 K (minus 389 F), far warmer than the reigning niobium-tin superconductors, which become superconducting at 18 K (minus 427 F). The higher T_c of MgB_2 also makes cooling the material more economical as it allows for the use of inexpensive refrigerators in place of liquid helium.

Magnesium diboride's unexpected

superconducting capabilities generated speculation about the material's potential for replacing niobium-tin superconductors in various applications, thus reducing the expense of those technologies. But for that speculation to become a reality, more basic research was needed to increase both the magnetic field MgB$_2$ can withstand and the electric current it can carry. Now, Ames Laboratory physicists Paul Canfield, Sergey Bud'ko and Doug Finnemore and graduate assistant Derek Wilke have done just that.

Perturbed to new heights

Canfield, who is also an Iowa State University physics professor, and his group were the first to describe the mechanism of superconductivity in MgB$_2$. They also devised a method of turning boron of a given form into MgB$_2$ with a similar form by allowing magnesium vapor to diffuse into the boron matrix. This patented technique has been used to make pellets, wire segments and thin films. Their familiarity with MgB$_2$ serves the researchers well in current efforts to enhance its superconducting properties.

"In this game, once you get an idea of what the pure material is doing, you want to perturb it," Canfield says. "You want to mess with it and see how it responds. The problem is that it's very hard to systematically perturb MgB$_2$. It really wants to form in a fundamentally pure fashion."

As it turns out, "messing" with the material is one of the things Canfield and his group do best. They were able to figure out how to get carbon into MgB$_2$. Experiments done by Wilke showed that a 5 percent substitution of boron with carbon more than doubles the magnetic field MgB$_2$ can withstand and still remain superconducting, raising it from 16 Tesla for the pure material to 36 Tesla. Even though the carbon-doping of MgB$_2$ lowers its critical temperature to 35 K (minus 397 F), 4 K less than in the pure material, the magnetic field as a function of temperature exceeds any of the NbSn compounds, which "peak out at around 30 Tesla," according to Canfield. "That sounds promising, but there are two things still out there that need to be resolved," he cautions.

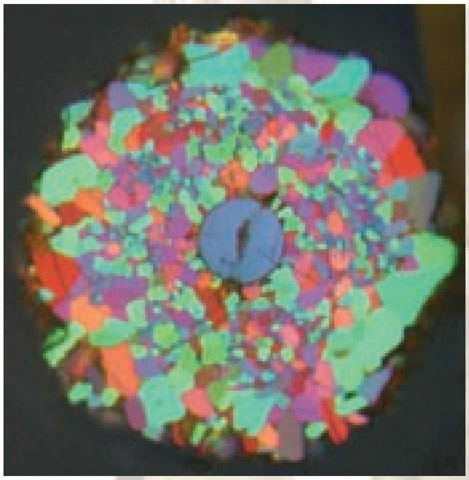
"One is determining how much current you can pass through the material and still have it remain superconducting," Canfield continues. "That's the critical current, and it's still inferior to Nb$_3$Sn."

Entrapping electrons

Increasing the critical current that MgB$_2$ can withstand and still remain superconducting is a challenge because whenever large electric currents pass through a superconductor, tiny whirlpools of electrons, called vortices, are created. The motion of these vortices saps energy and degrades a material's ability to superconduct. Finnemore's specialty is pinpointing the locations of electron vortices, and knowing their locations makes it possible to "pin" them.

If electrical and magnetic conditions are right, vortices will stick, or pin, themselves to nanometer-size precipitates in a superconductor. Once pinned to these impurities, they no longer move or dissipate energy. The trick is to find just the right impurity that will trap the vortices yet still allow the electricity to flow through the material.

"Titanium diboride is our first try as a precipitate, and it works without sucking out the carbon we added to increase the magnetic field," says Finnemore. He and Wilke added the TiB$_2$ using chemical vapor deposition, which disperses the element uniformly throughout the material. "We think it's just a better way to make samples than mixing powders," Finnemore adds. "Over the next few years, we hope to try other precipitates using chemical vapor deposition."



The image is a cross section of a 5 percent carbon-doped wire taken with polarized light. The picture shows the small, ~10-micron-sized grains lit up in brilliant colors.

Although Canfield is pleased with his group's success in enhancing the superconducting properties of MgB$_2$, he's cautious about predicting too much too soon in terms of the material replacing Nb$_3$Sn. He reminds us that there's still that "second thing" out there that needs to be resolved.

"Even if we can tweak the critical current to be better or comparable to Nb$_3$Sn, there's still the metallurgy of determining how to get a sheath around this material and make it a useful wire rather than just a lab sample," Canfield says. "That's just beyond anything we do as basic physicists; it will have to happen on some engineering time scale. But as far as temperature and critical field go, it's now looking better than Nb$_3$Sn on both of those parameters. Now, the critical current needs to be comparable or better."

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Materials Science and Engineering Division

Science to the Extreme

by Robert Mills

R. Bruce Thompson (right) demonstrates nondestructive evaluation techniques to two 8th-grade students at Southeast Polk Junior High. To the students' left are Iowa Governor Tom Vilsack and Sylvia Clark, executive director of the NEC Foundation of America.

The director of the Ames Laboratory's Nondestructive Evaluation Program, R. Bruce Thompson, was one of the scientists selected to participate in NEC Extreme Science in spring of 2004. This program, organized by the NEC Foundation of America, brings together middle-school students and teachers with America's most accomplished scientists and engineers to introduce students to the wonders of science and technology. Thompson, who is also a distinguished professor of engineering at Iowa State University, was selected to participate because of his membership in the National Academy of Engineering.

Along with Iowa Governor Tom Vilsack and Silvia Clark, executive director of the NEC Foundation, Thompson visited Southeast Polk Junior High School in Runnells, Iowa, and Woodrow Wilson Middle School in Council Bluffs, Iowa. Thompson used real-world examples and hands-on demonstrations to give the students a glimpse into the world of nondestructive evaluation. Covering topics such as acoustic waves, why materials fail, metal fatigue and accident investigation, Thompson showed how the technology is applied to detect and prevent failures in structures such as bridges, planes and pipes.

According to the Council Bluffs *Nonpareil* newspaper, Woodrow Wilson 8th-grade teacher Ed Stacy said the visit was a wonderful opportunity for his students to get a firm grasp on science. "With this opportunity, kids are able to get the fact that science is real and is all around them."

The NEC Foundation of America was established in 1991 and endowed at $10 million by NEC Corporation and its U.S. subsidiaries.

The Road to Lindau

by Saren Johnston

For Deborah Zorn, the road to Lindau, Germany, and the 54th International Convention of Nobel Laureates began in childhood. The Ames Laboratory graduate student from Lincoln, Neb., says she rarely missed an airing of Public Television's "Newton's Apple" and almost always took summer science classes in Lincoln's Bright Lights program.

Zorn is one of 25 top, young researchers from the United States who received full support from the DOE's Office of Science to attend the June 27-July 2 Lindau meeting. There, she interacted with Nobel Laureates and networked with student participants from around the world.

"Debbie is interested in all aspects of science and is fearless and successful in attacking problems," says Mark Gordon, Zorn's major professor and director of Ames Laboratory's Applied Mathematics and Computational Sciences Program.

Zorn studies theoretical and computational chemistry at Iowa State University. In one DOE research project, she is creating and implementing theoretical and computational models to ease the identification of properties in new materials being developed for catalytic systems.

Another of Zorn's DOE projects uses quantum mechanics and molecular mechanics methods to study the behavior of certain metals on a silicon surface. The work may lead to atomic wires one atom wide for nanotechnology applications.

Zorn credits her father with encouraging her interest in science. "He instilled an interest in science and an appreciation for math in me for which I will always be grateful," she says.

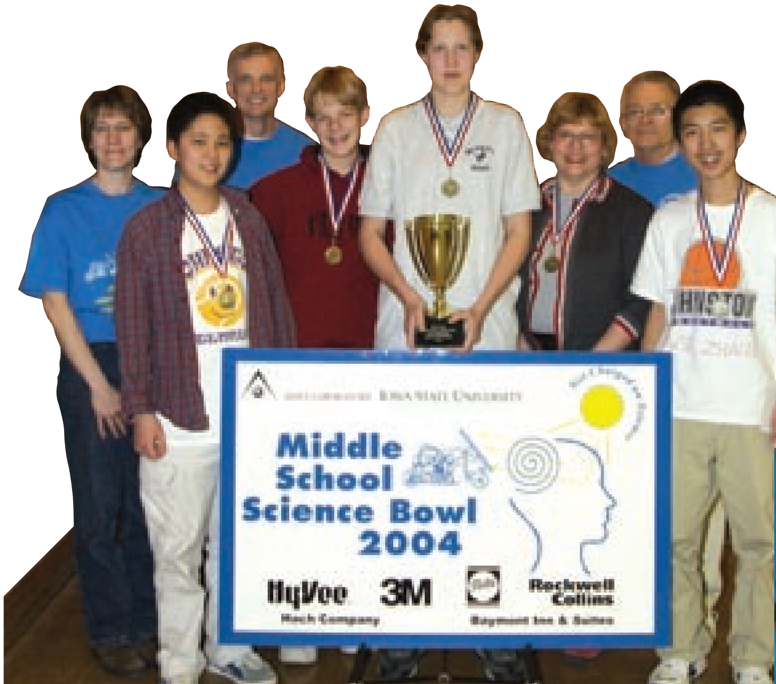
Science is Zorn's passion, but she's also an art enthusiast and an accomplished golfer, earning NCAA division III All-American and Academic All-American Athlete honors.

"I like to think of myself as a creative person," says Zorn. "Whether it's science, art or sports, it's all about problem-solving. I enjoy taking bigger problems and breaking them down until they are similar to something I've seen before and that I can solve."

Double the Science Bowl Fun

Ames Lab Adds Middle School to the Mix

by Steve Karsjen



Central Academy of Des Moines, Iowa, took top honors in the academic competition portion of Ames Laboratory's first-ever Middle School Science Bowl.

After 14 successful years of stirring up enthusiasm for science with its annual Regional High School Science Bowl, Ames Laboratory spiced things up even more by adding a middle school event to the mix in 2004.

Sixty students, their coaches and parents from 10 Iowa and two Minnesota middle schools traveled to the Iowa State University campus to help launch Ames Laboratory's first Middle School Science Bowl, April 23-24. The two-day event included building and racing hydrogen fuel-cell cars and a quiz-bowl-style competition.

Opening comments from Larry Jones, an Ames Laboratory associate metallurgist who served as science advisor for the Middle School Science Bowl, and presentations on solar energy and hydrogen fuel cells by members of ISU's solar car club, Team PrISUm, prepared students for the much anticipated car-construction and car-racing activity on the first day of competition.

Why haven't we always used fuel cells? Are all fuel cells the same size? Aren't solar cells expensive? These were just some of the many questions Jones and Team PrISUm members fielded from the attentive and enthusiastic middle school students.

Once given the OK, it didn't take long for the students to get their car kits opened and the parts laid out on the tables. "I think this goes here," and "No, it goes here – let me show you," were comments repeated frequently as the students assembled the myriad of wires, tubes and other parts to build the cars. Not surprisingly, with just a little help from Team PrISUm, Jones and other volunteers, the students had the hydrogen fuel-cell cars assembled in no time at all.

During the construction process, volunteers helped the students understand how to operate the cars on solar power. The students learned how solar power can be used to split water molecules to create both hydrogen and oxygen gas and also how the combining of hydrogen and oxygen in a fuel cell can generate electricity that can be used to power a car's motor.

Surrounded by members of Team PrISUm, Central Academy students prepare their car for the start of a race.

At the end of the day, the student team from Miller Middle School in Marshalltown, Iowa, took top honors in the fuel-cell car challenge. "My son said it was his best day ever," said one appreciative parent about the fuel-cell car challenge.

The second day of the Middle School Science Bowl brought a full day of academic competition. At the end of the day, Des Moines Central Academy, Des Moines, Iowa, won the quiz-bowl part of the competition. "Obviously, we were saving all of our brain power for today," chuckled the Central coach, referring to her team's loss in the previous day's fuel-cell car challenge.

The inaugural Middle School Science Bowl drew rave reviews from the participants. Many of the students made a special point of telling competition organizers how much they enjoyed the two-day event. Said the coach from Ordean Middle School in Duluth, Minn., "We'd love to come back."

Inquiry 2004

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Ames Laboratory is a U.S. Department of Energy laboratory seeking solutions to energy-related problems through the exploration of chemical, engineering, materials and mathematical sciences, and physics. Established in the 1940s with the successful development of the most efficient process to produce high-purity uranium metal for atomic energy, Ames Lab now pursues much broader priorities than the materials research that has given the Lab international credibility. Responding to issues of national concern, Lab scientists are actively involved in innovative research, science education programs, the development of applied technologies and the quick transfer of such technologies to industry. Uniquely integrated within a university environment, the Lab stimulates creative thought and encourages scientific discovery, providing solutions to complex problems and educating tomorrow's scientific talent.

AMES LABORATORY A U.S. Department of Energy laboratory operated by Iowa State University