INQUIRY | 2006

SCIENCE & TECHNOLOGY AT THE AMES LABORATORY

Nanoscale Drug Delivery

· Digital Detective Work

· Beauty Near Absolute Zero

· Marvelous Metamaterials

AMES LABORATORY

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

INQUIRY

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, Ames Laboratory 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.

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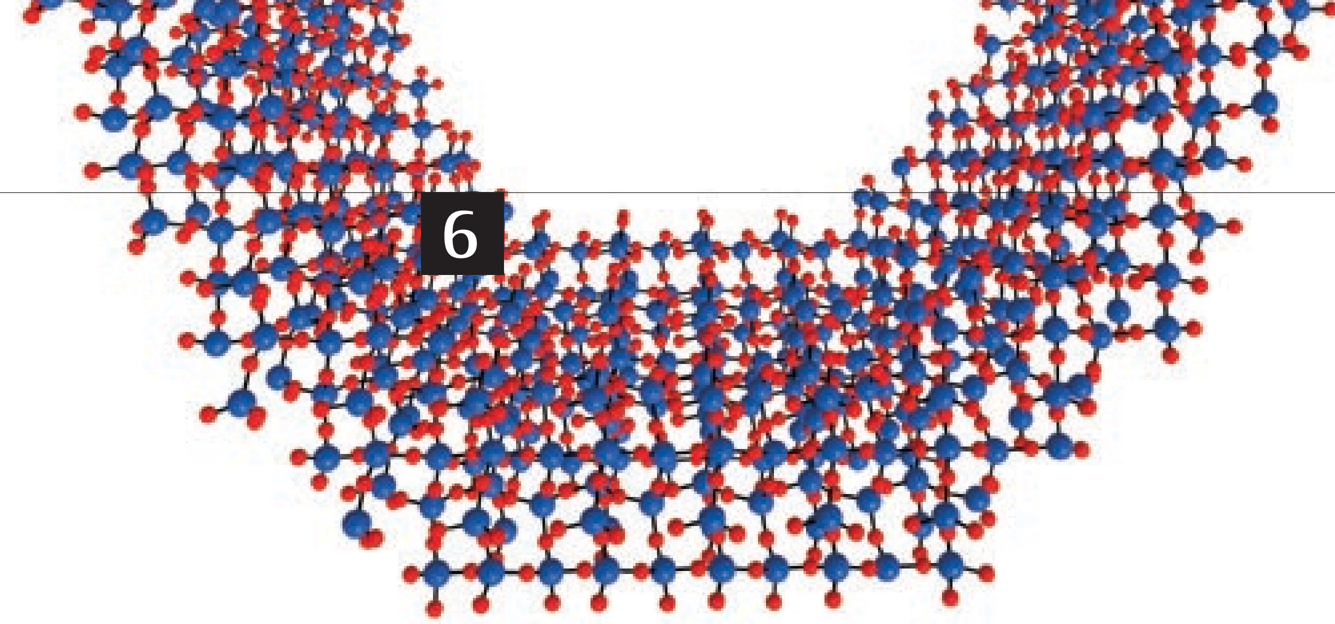

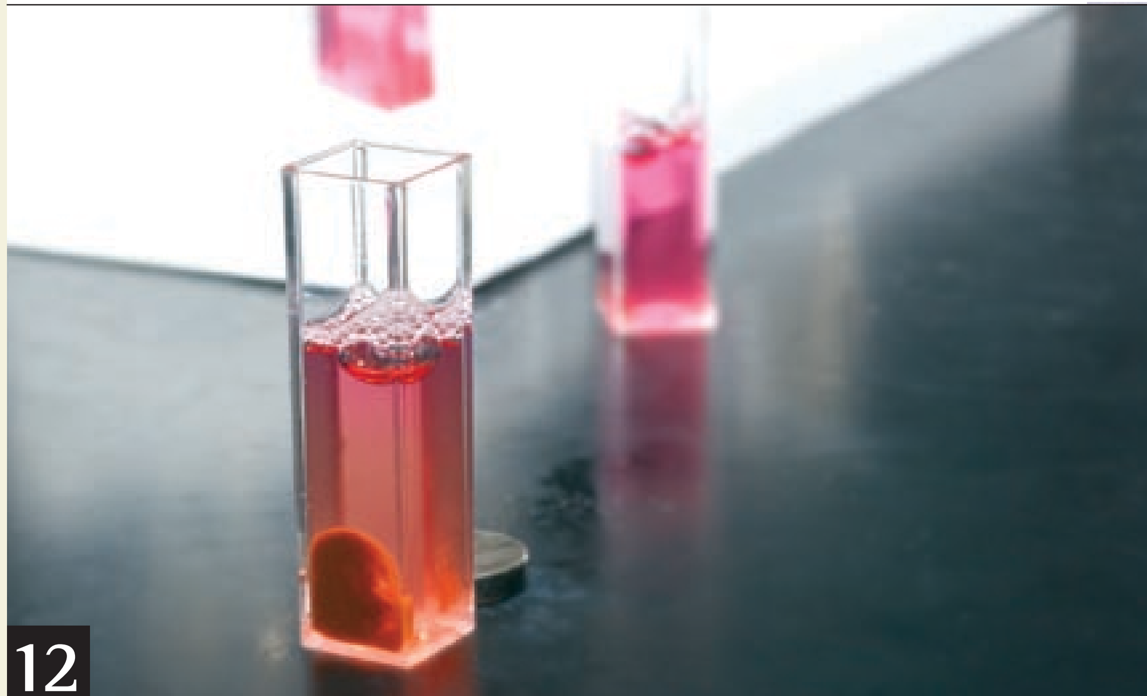

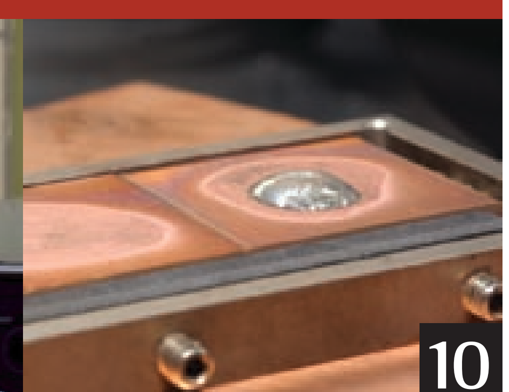

Cover photo: *A micrograph of chemist Victor Lin's mesoporous silica nanoparticles shows the tiny channels that can be filled with drugs that are released once the particles are absorbed by living cells.*

Back cover: *A glass condenser coil catches and reflects laboratory lights.*

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From the Director

WELCOME TO THE 2006 ISSUE OF *Inquiry* magazine. As I write this in early August, the clock is ticking down on the competitive bidding process for operation of Ames Laboratory. It's the first time in the nearly 60-year history of the Lab that the Department of Energy will consider potential contractors besides Iowa State University, the Lab's exclusive contractor since its inception. By the time you read this, the bidding process will be completed.

While the outcome of that process is unknown at this point, one thing is crystal clear – the quality of the research at Ames Laboratory continues to be world-class. For the second straight year and the 16th time overall, Ames Laboratory researchers have received an R&D100 Award. Mark Bryden, Gerrick Bivins, and Doug McCorkle have created software that takes large 3-D data sets and quickly converts them into images with which engineers can analyze and work. The software has been used to study ways to reduce emissions from power plants, decrease pollution from swine confinements and improve vehicle efficiency – the possibilities are almost limitless. You can read more about this exciting work in the Bryden group on the opposite page.

Senior physicist Costas Soukoulis won international recognition in December, coordinating a multinational team that received the Descartes Prize for Excellence in Scientific Collaborative Research, the European Union's highest honor in the field of science. He and his collaborators received the prestigious award for creating a novel class of artificial metamaterials called left-handed materials, which exhibit negative refraction, bending light in the opposite direction to that seen in natural materials. You'll find information on Dr. Soukoulis' award and pioneering work on Pages 9 and 20.

Chemist Victor Lin continues to find exciting uses for tiny particles of silica – mesoporous nanoparticles. His latest effort utilizes them to deliver drugs within living cells and selectively release their pharmaceutical payload so that only targeted cells benefit from the drug while healthy cells are left unaffected. You can see the system in action beginning on Page 14.

One of the long-standing mysteries in organic chemistry – a field close to my heart – is the nature of the mechanism that triggers the Fenton reaction, one of the most powerful oxidizing reactions available for breaking apart organic compounds. Ames Lab senior scientist Andreja Bakac and her collaborators at two other universities, were able for the first time to produce and study a novel compound containing iron and effectively rule out its frequently speculated involvement in the Fenton reaction. Dr. Bakac's work is detailed on Page 12.

Ames Laboratory's education efforts continue to benefit the young people of Iowa and students from around the country. Teams from our Regional Middle School and High School Science Bowl competitions both finished in the prize money at their respective national contests, competing against often much larger schools from around the country. Our Science Undergraduate Laboratory Internship, or SULI, program brought another 10 undergraduate students from all over the United States to work closely with Ames Lab and Iowa State University research mentors in a variety of disciplines.

And we've initiated a Laboratory Science Teacher Professional Development, or LSTPD, program that will bring 10 middle school teachers from Iowa, Minnesota and South Dakota to the Lab to participate in the Teachers as Investigators program starting next summer. Through the program, teachers will conduct hands-on, discovery-based experiments with advanced equipment right here at the Lab and then learn how to bring exciting breakthroughs and frontiers of science into their classrooms.

As the research projects detailed in the pages of *Inquiry* demonstrate, Ames Laboratory is committed to finding solutions through innovative science. I hope that you enjoy learning about some of our recent successes, as well as our efforts to ensure that our country has outstanding scientists for the future.

Bryden, Bivins and McCorkle Win 2006 R&D 100 Award

BY SAREN JOHNSTON

(left to right) Doug McCorkle, Mark Bryden and Gerrick Bivins.

Award brings Ames Lab's total to a "Sweet 16"

A TEAM OF AMES LABORATORY AND IOWA STATE University researchers has won a 2006 R&D 100 Award for their development of a novel software engineering tool that greatly eases the problem-solving and decision-making processes for engineers. Their software tool, Texture Based Engineering Tools, or TBET, provides engineers an unrivaled means of interacting with large 3-D data sets to tackle complex engineering projects. The award-winning work has been supported by close to $1.3 million from the Ames Laboratory.

TBET is the brainchild of Ames Laboratory scientist Kenneth "Mark" Bryden, who is also the Iowa State University associate chair of mechanical engineering and an associate professor in that department. Co-developers are Gerrick Bivins, an ISU assistant scientist working in Bryden's lab, and Douglas McCorkle, an ISU mechanical engineering doctoral student. Their win of a 2006 R&D 100 Award brings the Laboratory's total to 16 since 1984.

The winning of an R&D100 Award provides a mark of excellence known to industry, government and academia as proof that the product is one of the most innovative ideas of the year.

Applauding the Ames Lab and ISU accomplishment, Secretary of Energy Samuel W. Bodman said, "I congratulate the researchers who have won this award, which highlights the power and promise of DOE's investments in science and technology. Through the efforts of dedicated and innovative scientists and engineers at our national laboratories, DOE is helping to enhance our nation's energy, economic and national security."

Present at Birth: *The award-winning Texture Based Engineering Tools, TBET, allows Doug McCorkle (left) and Gerrick Bivins to enter a virtual environment that displays velocity information from a data set about the birth of a star.*

Echoing the Secretary's praise, Ames Laboratory Director Tom Barton says, "The innovative, pioneering work coming from Mark Bryden and his research group is changing the way engineers can manage huge amounts of interactive data to maximize design and operational efficiency. The Ames Laboratory is proud to play this role in aiding American industry to maintain world-class competitiveness."

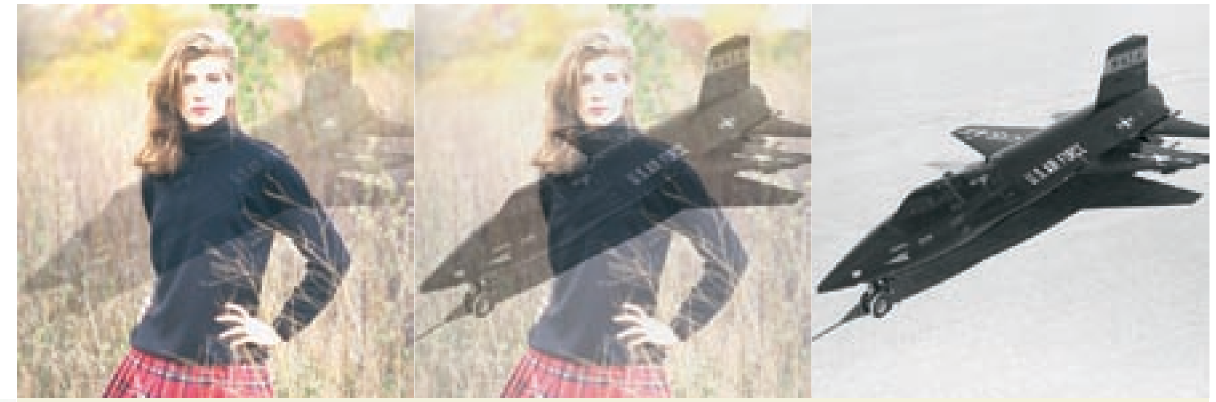
Bryden says that Texture Based Engineering Tools is one component of an open-source engineering software package called VE-Suite that enables virtual engineering to take place. "There is nothing on the market that can do the job as quickly and intuitively," Bryden emphasizes.

The John Zink Company LLC, a recognized leader of advanced pollution-controlled systems, fire equipment and next-generation technologies, is taking advantage of TBET's unique visualization capabilities in their efforts to improve designs of combustion systems.

"The Texture Based Engineering Tools that are implemented in VE-Suite are critical to helping our engineers gain unparalleled insights into the computational fluid dynamics models of combustion systems," says Christopher Jian, director of simulation technology solutions for John Zink.

Bryden, Bivins and McCorkle will be honored for their development of Texture Based Engineering Tools at the R&D 100 Awards Banquet, Oct. 19, in the Grand Ballroom of Chicago's Navy Pier. Their TBET technology will be among the 2006 R&D100 winners featured in the September issue of *R&D Magazine*.

Bryden says one of the best things about winning an R&D100 Award is that it spreads the word about virtual engineering and helps people better understand the process.



The images shown opposite and above represent how ever-increasing amounts of the payload file – the fighter jet – are embedded in the original image. In actual use, the changes in the original image are so subtle that it's impossible to tell that the image has been altered.

Hiding in Plain Sight

Researchers detect secret files lurking within digital images

BY KERRY GIBSON

KEEPING COMPUTER FILES PRIVATE REQUIRES only the use of a simple encryption program. For criminals or terrorists wanting to conceal their activities, however, attaching an encrypted file to an e-mail message is sure to raise suspicion with law-enforcement or government agents monitoring e-mail traffic.

But what if files could be hidden within the complex digital code of a photographic image? A family snapshot, for example, could contain secret information, and even a trained eye wouldn't know the difference.

That ability to hide files within another file, called steganography, is here thanks to a number of software programs now on the market. The emerging science of detecting such files – steganalysis – is getting a boost from the Midwest Forensics Resource Center and a pair of Iowa State University researchers.

Payloads and JPEGs

Electronic images, such as JPEG files, provide the perfect "cover" because they're very common – a single computer can contain thousands of JPEG images, and they can be posted on Web sites or e-mailed anywhere. Steganographic, or stego, techniques allow users to embed a secret file, or payload, by shifting the color values just slightly to account for the "bits" of data being hidden. The payload files can be almost anything from illegal financial transactions and the proverbial off-shore account information to terrorist-cell communications or child pornography.

"We're taking very simple stego techniques and trying to find statistical measures that we can use to distinguish an innocent image from one that has hidden data," says Clifford Bergman, an ISU math professor and a researcher on the project. "One of the reasons we're focusing on images is there's lots of 'room' within digital images to hide data. You can fiddle with them quite a bit, and visually a person can't see the difference."

"At the simplest level, consider a black and white

Seemingly innocent images can be used to hide other computer data by using steganography programs that replace bits of information in the original image with encrypted data from the payload file.

photo – each pixel has a grayscale value between zero (black) and 255 (white)," says Jennifer Davidson, an ISU math professor and the other investigator on the project. "So the data file for that photo is one long string of those grayscale numbers that represent each pixel."

Encrypted payload files can be represented by a string of zeros and ones. To embed the payload file, the stego program compares the payload file's string of zeros and ones to the string of pixel values in the image file. The stego program then changes the image's pixel values so that an even pixel value represents a zero in the payload string and an odd pixel value represents a one. The person receiving the stego image then looks at the even-odd string of pixel values to reconstruct the payload's data string of zeros and ones, which can then be decrypted to retrieve the secret file.

"Visually, you won't see any difference between the before and after photo," Davidson says, "because the shift in pixel value is so minor. However, it will change the statistical properties of the pixel values of the image, and that's what we're studying."

Artificial intelligence

Given the vast number of potential images to review and the variety and complexity of the embedding algorithms used, developing a quick and easy technique to review and detect images that contain hidden files is vital. Bergman and Davidson are utilizing a pattern-recognition system called an artificial neural net, or ANN, to distinguish between innocent images and stego images.

Training the ANN involved obtaining a database of 1,300 "clean" original images from a colleague, Ed Delp, at Purdue University. These images were then altered in eight different ways using different stego embedding techniques – involving sophisticated transfer techniques between the spatial and wavelet domains – to create a database of over 10,000 images.

Once trained, the ANN can then apply its rules to new candidate images and classify them as either innocent or stego images.

"The ANN establishes kind of a threshold value," Bergman says. "If it falls above the threshold, it's suspicious."

"If you can detect there's something there, and better yet, what method was used to embed it, you could extract the encrypted data," Bergman continues. "But then you're faced with a whole new problem of decrypting the data … and there are ciphers out there that are essentially impossible to solve using current methods."

In preliminary tests, the ANN was able to identify 92 percent of the stego images and flagged only 10 percent of the innocent images, and the researchers hope those results will get even better. An investigator with the Iowa Department of Criminal Investigation is currently field-testing the program to help evaluate its usefulness, and a graphical user interface has been developed to make the program more user-friendly.

"Hopefully we can come up with algorithms that are strong enough and the statistics are convincing enough for forensic scientists to use in a court of law," Bergman says, "so they can say, 'There's clearly something suspicious here,' similar to the way they use DNA evidence to establish a link between the defendant and the crime."

The Midwest Forensics Resource Center, operated by Ames Laboratory and Iowa State University, provides research and support services to crime laboratories and forensic scientists throughout the Midwest.

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The Computational Chemistry "Toolbox"

BY SAREN JOHNSTON

Turning sophisticated theory into scalable code

YOU NEED THE RIGHT TOOLS FOR THE job at hand. It's a familiar phrase. We hear some version of it every day in all forms of advertising, from newspaper ads to television commercials to unwanted e-mails. The sales pitch is a popular one, mostly because the reality is pretty much undeniable: using the appropriate tools for a specific task almost always results in time-, energy- and cost-savings.

No need to tell this to Mark Gordon – you'd be preaching to the choir. Gordon, director of Ames Laboratory's Applied Mathematics and Computational Sciences program and an Iowa State University Distinguished Professor of chemistry, has devoted much of his career to making sure the right tools are available in GAMESS, the "toolbox" that he and thousands of researchers worldwide use on a daily basis to learn more about the goings-on of molecules and atoms – how they act, interact and react.

GAMESS, or the General Atomic and Molecular Electronic Structure System, is a software suite chock-full of quantum chemistry codes and functionalities – the tools that significantly enhance efforts focused on finding solutions to problems involving molecular processes, such as designing new fuels and gaining better insights into combustion, catalysis and photochemical energy conversion.

Gordon fosters the development of GAMESS and its software tools, which continue to grow and diversify as a result of his contributions to the suite and those of many other "code crafters," including Gordon's co-worker, Ames Lab associate Mike Schmidt, various current and past members of the Gordon research group, and numerous professional colleagues.

The GAMESS software tools are designed to take advantage of parallel, high-performance supercomputing systems that are capable of doing trillions of calculations per second. On such systems, the versatile software suite can perform the very highest levels of theory for modeling complex physical, chemical and biological systems. The continued enhancements Gordon and his colleagues make to GAMESS dramatically improve the ability to do such high-end and accurate calculations, a feat that at first glance may seem to impact only a select few. However, Gordon promptly rejects this all-too-quick assumption.

"If you have something that's the highest level of theory you can do, and you make that better in some way – faster, more convenient, more accurate – that has an impact on your ability to say, 'We've nailed this now, and now other people can use this as a benchmark for simpler methods,' " explains Gordon.

"Toning up" the toolbox

Helping advance the capability to do top-notch theory is an enhancement to the GAMESS toolbox that combines the Fragment Molecular Orbital, or FMO, method of handling large molecular systems quantum mechanically with the Polarizable Continuum Model, or PCM, for solvent computations. Now that's a lot of technical talk, so let's see if we can break it down.

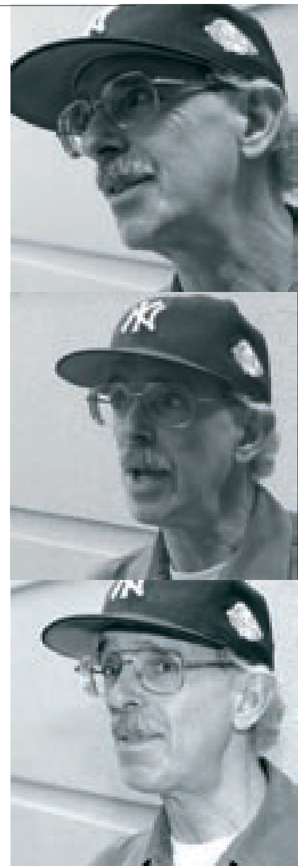
Interestingly, breaking it down is exactly the idea behind the FMO portion of this combination tool. Gordon explains, "What you'd like to do, in principle, is take the highest level of theory you can do and apply it to a big molecule, such as a polymer, enzyme or protein. The problem is that to do quantum chemistry on something that big is hugely expensive computationally, especially if you want to do a level of theory that is very demanding. The FMO method offers a way of 'chopping' a very large molecule into relatively small pieces by doing explicit calculations on monomers, the repeat units in a polymer, and dimers, which are two monomers. Some very clever methods are then used to put all those fragments together to make the larger system."

> "There is a great satisfaction in building good tools for other people to use."
>
> ~FREEMAN DYSON, English-born American physicist and mathematician

But how good is the piecing together of fragments relative to doing the full calculation if you could do the full calculation? Gordon says test calculations can be done on small molecules in which the full calculations can be accomplished without any approximation. These calculations can then be compared to those derived from the molecule's FMO. "The errors are within what most people call chemical accuracy," he notes. "The way to think about this is if an experimentalist had error bars, then the accuracy would be within those error bars and would never impact the experiment. And that's pretty good!"

Gordon credits his former graduate student, Dimitri Fedorov and his colleague Kazuo Kitaura, both of the Japanese National Computational Laboratory, AIST, for developing the FMO method for the GAMESS software suite. "The FMO method has been implemented for five different levels of theory, from the very lowest level of quantum chemistry theory that we do to the very highest," he says. "Fedorov and Kitaura are interested in biomolecules, so they've done calculations on systems with as many as 20,000 atoms, which is unheard of in quantum chemistry. You're lucky if you can do 100 atoms with quantum chemistry, so this is orders of magnitude larger than what people can usually do."

Adding water to the tool "pool"



Mark Gordon

Making a good tool even better, Gordon led a team that included his postdoctoral research associate, Hui Li; former graduate student Jan Jenson, now at the University of Iowa; Fedorov; and Kitaura in developing a method of modeling the activity of molecules in solution. They created the new GAMESS tool by interfacing the Polarizable Continuum Model, PCM, with the FMO method. "If you're interested in polymers and enzymes, whatever they do, they do in solution, usually in aqueous solution," says Gordon. "That means just doing FMO calculations is not enough – you need to get the solvent in there." Expanding, he says, "If you imagine a solvent and throw in something like a protein, the protein sort of sweeps out a volume. We're not looking at individual water molecules now – we're representing the whole solvent sort of as a sea." Offering an analogy, he continues, "It's exactly as if you went swimming. You don't see the individual water molecules; you see the whole ocean. So that's the nature of this type of method, and we have a very nice one in GAMESS."

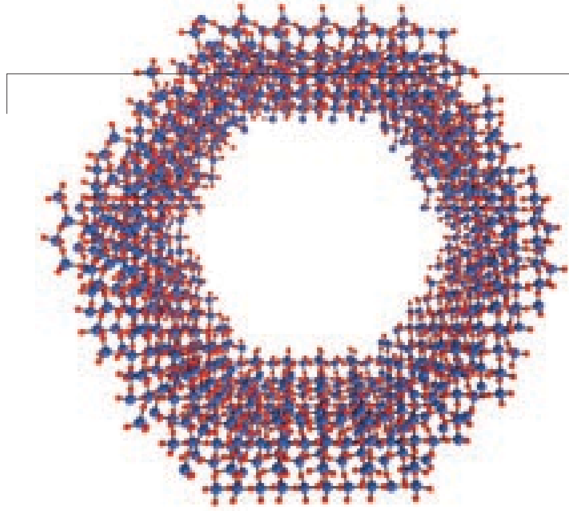
A tool of prediction

A GAMESS tool that has been around since 1990 and continues to be improved upon is the Effective Fragment Potential, or EFP. When scientists deal with systems containing so many atoms that quantum mechanics can't be done, even at simple levels, the EFP method offers an alternative means. By combining the EFP with quantum mechanics in a way that a quantum mechanical description is produced only for that portion of a system that is going through a chemical change, scientists can then approximate the remainder of the system based on that fragment of information. The entire calculation takes orders of magnitude less time than a fully quantum calculation.

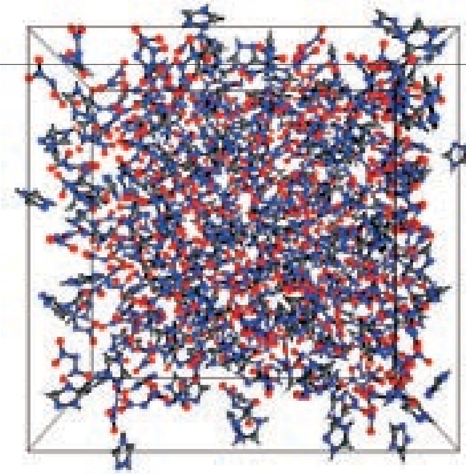
"The effective fragment potential is becoming more and more exciting as we try to model the interactions between molecules," says Gordon of the method that he and Jan Jenson developed in collaboration with Dr. Walter Stevens at the National Institute of Standards and Technology.

"This time we do care about each water molecule or each solvent molecule," Gordon notes. "Molecules interact with each other in a variety of different ways, and some of those interactions are easier to derive models for than others."

Some molecular interactions that are not so easy to model are those associated with dispersion and charged



MacMolPlt, a GAMESS tool developed by Ames Lab associate scientist Brett Bode, makes it possible to visualize the results of GAMESS calculations on Macintosh computers. The above MacMolPlt image is of a mesoporous silica nanopore. Mesoporous silica materials hold great promise for the design of a new generation of highly efficient and selective catalysts.



This image is a molecular dynamics simulation of an ionic liquid composed of 512 ions. There are 256 positively charged ions (1,2,4-triazolium) and 256 negatively charged ions (dinitramide). The simulation was done on a 16-CPU parallel machine using the new GAMESS effective fragment potential code. The CPU time efficiency was 96 percent – testimony to the efficiency of the innovative GAMESS tool.

species. Nonetheless, Gordon and his group members have added those capabilities to GAMESS in the past year.

Dispersion

Dispersion is one means by which molecules exert forces on one another. Dispersion forces are randomly and spontaneously generated continuously over the entire molecule, making them extremely difficult to model. However, Ivana Adamovic, a former Gordon group member now at the Harvard School of Health in Boston, took on the challenge, developing a model potential for GAMESS that handles this fleeting molecular ebb and flow. Thanks to her contribution, the Gordon group has been able to use the new GAMESS tool to do calculations on DNA base pairs, and they are currently working with the ISU chemical engineering department to study the aggregation of polymers, such as latex.

Charge transfer interactions

Charge transfer interactions are those that occur between ions. Ionic bonds are formed when the relationship between two atoms or molecules is such that one of them has a far greater ability to attract electrons and "steals" an electron from the other so that the now oppositely charged ions are attracted.

Hui Li, who will be an assistant professor at the University of Nebraska in the fall of 2006, and Heather Netzloff, a former graduate student of Gordon's now at Australian National University, enhanced the EFP method for GAMESS by respectively creating a molecular dynamics code to address the interactions that occur between ions and optimizing the code to take advantage of parallel computers.

The addition of the charge transfer code to the GAMESS toolbox is of particular importance to Gordon who is interested in ionic liquids in the design of high-energy fuels — products that bring together positively and negatively charged species. "You can't simulate those relationships adequately unless you have something that accounts for the charge transfer interactions, and we now have in GAMESS a molecular dynamics code that allows us to do that thanks to Hui and Heather," says Gordon.

The "tool" de force

"GAMESS runs on every kind of computer platform and compiler you can imagine," says Gordon. "It just passed 20,000 registered user groups in over 100 countries. This translates into an estimated 100,000 to 150,000 individual users. They range from people in academics to industry to government labs."

GAMESS is distributed at no cost to users by accessing *www.msg.ameslab.gov* and signing a license agreement.

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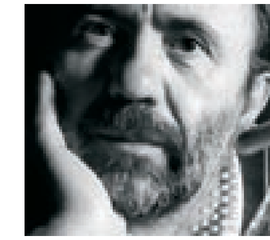
Costas Soukoulis Wins European Union's Highest Science Prize

BY SAREN JOHNSTON

Costas Soukoulis accepts the 2005 Descartes Prize for Excellence in Scientific Collaborative Research at the Royal Society in London on Dec. 2. Members of the winning collaborative team are, left to right: Stephan Linden (University of Karlsruhe), Mike Wiltshire (Imperial College), Maria Kafesaki (FORTH), David Smith (Duke University), Martin Wegener (University of Karlsruhe), Ekmel Ozbay (Bilkent University), and Sir John Pendry (Imperial College).



Costas Soukoulis

COSTAS SOUKOULIS, an Ames Laboratory senior physicist and an Iowa State University Distinguished Professor of physics and astronomy, coordinates the research team that won the 2005 Descartes Prize for Excellence in Scientific Collaborative Research, the European Union's highest honor in the field of science. He and his collaborators received the prestigious award for creating a novel class of artificial metamaterials called left-handed materials, or LHMs, which exhibit fascinating properties that cannot be found in naturally occurring materials.

LHMs exhibit negative refraction, bending light in the opposite direction to that seen in natural materials. They can be fabricated to have zero reflectance for all angles hit by incoming electromagnetic waves. In addition, they can focus light without the need for curved surfaces. These and other amazing properties promise a wide range of potential applications for LHMs.

Soukoulis, who has also been an associate with the research center FORTH, in Crete, Greece, since 1984, said he was lucky to work with a top-notch team of international researchers in creating the new subclass of materials. The team includes Professor Sir John Pendry, Imperial College, UK; Professor Ekmel Ozbay, Bilkent University, Turkey; Professor Martin Wegener, University of Karlsruhe, Germany; Professor David Smith, Duke University, USA; and Professor E. N. Economou and Dr. Maria Kafesaki, both from FORTH and the University of Crete.

The research team was awarded the Descartes Prize for Research in Physics at a ceremony held at the Royal Society in London on Dec. 2, 2005. The team received prize money of 1 million euros (about $1.3 million) for their winning project, "Extending Electromagnetism through Novel Artificial Materials, or "EXEL."

"Our EXEL team was able to demonstrate the experimental reality of LHMs and their consistency with the laws of physics," said Soukoulis. "This realization opened up the possibility of unprecedented applications and devices."

The team has already shown how the ability to focus radio waves could lead to smaller, better-performing magnetic resonance imaging machines for medical diagnostics. Numerous applications in the cellular communications industry are also envisioned, including antennas and waveguides that are 100 times smaller and much lighter than those of today. Even slight improvements to these types of devices can make a significant financial impact.

Ames Laboratory Director Tom Barton praised the work of Soukoulis and the EXEL team, saying, "It probably would be difficult to overstate the potential importance of this historic scientific achievement to the future of optical technology. The Ames Lab and Iowa State University are indeed proud of the pivotal role played by Professor Soukoulis."

Accepting the Descartes Prize, Soukoulis paid tribute to the organizations that have supported his research on LHMs. "I would like to express my gratitude to Ames Laboratory and Iowa State University for accommodating my teaching duties to allow me to also pursue research on left-handed materials in Europe," he said. "I would like to thank the U.S. Department of Energy for their support during the last 20 years. Our Ames Laboratory work on photonic crystals led to the field of negative index materials and metamaterials."

The Descartes Prize for Excellence in Scientific Research, now in its sixth year, recognizes outstanding scientific and technological results achieved through international collaborative research in diverse disciplines. Winners are selected by a grand jury of experts in science, industry and the general public.

Europe Lead-free

Thanks to Ames Lab Innovation

Lead-free solder licensed worldwide as EU lead-free rules take effect

BY KERRY GIBSON

LEAD HAS LONG BEEN RECOGNIZED AS A highly toxic material that can cause brain damage. Its use in paint was banned in 1978, and it was later removed from gasoline to further protect human health. But a burgeoning source – electronic waste – poses a substantial new threat to the environment as lead and other chemicals leach from computers, cell phones and other electronic devices being buried in landfills.

Effective July 1, the European Union began strictly limiting the amount of lead and other hazardous materials lurking within the circuitry of any electronic appliance sold.[1] Given the global nature of the electronics industry, however, the European ban is in essence international in scope. As electronics and appliance manufacturers scrambled to meet those tough new restrictions, a lead-free solder developed several years ago at Ames Laboratory played a key role.

Shiny glue

Solder is the shiny metallic "glue" that holds components on circuit boards and bonds other electrical connections. Though a computer's circuit boards contain only small amounts of lead solder, the problem is overall volume. By some estimates, about 3,000 tons of electronic waste is discarded daily just in the United States.

Composed of lead and tin, traditional solder melts and flows easily, but sets up quickly to create a strong, durable bond between the mating surfaces. A solder blend of 63 percent tin and 37 percent lead results in a eutectic alloy – one that acts like a pure metal with a single melting (and solidification) point.

"Finding a substitute for lead that gave the solder similar properties was difficult," says Ames Laboratory senior metallurgist Iver Anderson. "With our basic understanding of alloys, we developed a tin-silver-copper alloy that offered a lower melting temperature and greater strength than other lead-free alternatives being considered."

Big bucks

The Ames Laboratory's solder technology was patented in 1996, and nearly 60 companies worldwide have licensed Ames Lab's lead-free solder, according to Ken Kirkland, executive director of the Iowa State University Research Foundation. To date, those licenses have generated royalties in excess of $7 million. ISURF holds the patents for research developed at Iowa State, including Ames Laboratory.

"With the European directives and a similar commercial initiative in Japan, we've seen a growing interest in the alloy," Kirkland says. "The technology was a little ahead of its time, but it's an excellent product and we have a strong patent; you can't ask for a better combination than that."

The Ames Lab solder is just one of several lead-free alternatives on the market. The type and specific composition of lead-free solder also depends on the soldering technique used and the end application. In addition to the tin-silver-copper alloy, Anderson's group developed modified alloys that also contain iron, cobalt and other similar elements. These blends are suitable for higher-temperature applications and have also been patented by ISURF.

Battling brittleness

One ongoing problem with lead-free alternatives now available is their tendency to get brittle over time after repeated or prolonged heating cycles. And heat has become a growing factor as technological advances have boosted operating temperatures. For example, the steady climb in computer processor speeds has meant a corresponding increase in the amount of heat they generate. And computers aren't the only devices that generate heat.

"Even the circuitry in your cell phone operates at about 125 degrees Celsius," Anderson says, "and over six months' use, that can mean several hundred hours of high temperatures. If you drop it now, the solder joints have become more brittle and the risk of it 'breaking' is higher."

To combat this solder "aging" problem, Anderson's group has recently been studying more additives to the tin-silver-copper formula, including silicon, titanium, chromium, manganese, nickel, zinc and germanium. Joints soldered with the different alloys were subjected to 150 C for 1,000 hours, then tested for both shear strength and impact strength.

"Zinc appears to be most attractive in terms of retained ductility and strength," Anderson says, "and also offers benefits in terms of solderability, ease of alloying and material cost." While additional testing is needed, he adds that the tin-silver-copper-zinc composition is covered under the original patent.

Added bonus

One other benefit of this recent work is development of a simple technique for characterizing the bulk composition of solder joints using an electron microprobe. This permits Anderson's research team to analyze the new compositions being studied under different soldering conditions.

"With the elimination of lead, tin-silver-copper solders are here for the long run," Anderson says. "But that doesn't mean we'll stop trying to improve our basic understanding of how these alloys work in order to improve their performance."

[1] –*The Waste Electrical and Electronic Equipment directive and the Restriction of Hazardous Substances directive.*

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DOE Office of Basic Energy Sciences, Materials Science and Engineering Division

Cellular Drug Delivery from the Inside Out

BY KERRY GIBSON

IN THE 1966 SCIENCE-FICTION blockbuster, "Fantastic Voyage," a small submarine and its medical crew are miniaturized to microscopic size and injected into the body of a dying scientist. They journey through the man's body to remove a blood clot in his brain.

Fast forward 40 years. In a somewhat similar plot line, Ames Lab chemist Victor Lin has found a way to use nanoscale "capsules" to deliver a dose of chemotherapy drugs to specific cancer cells without the risk of side affects to healthy cells.

Using tiny silica particles called mesoporous nanospheres to carry drugs inside living cells, Lin is studying different methods to control whether the particle delivers its pharmaceutical payload.

"First, the nanospheres are only about 200 nanometers in diameter, roughly the size of a virus, so they won't trigger an immune response in the body," Lin says. "They're also biocompatible so they can be readily absorbed by the cells."

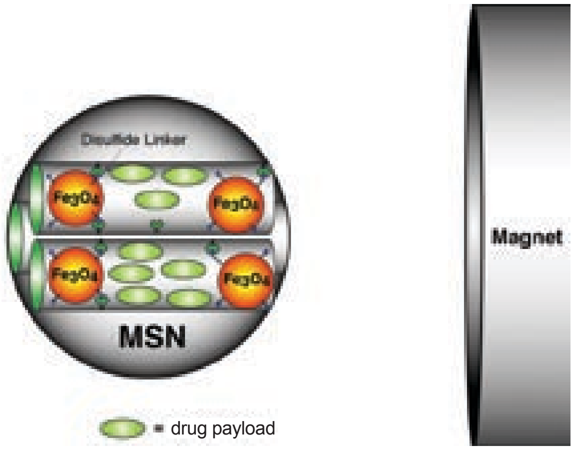
But it's the structure of the nanospheres that makes drug delivery possible. The spheres have thousands of parallel channels running completely through them. Through capillary action, the spheres can soak up molecules of the drug to be delivered. When the channels are filled, the ends of the channels are "capped" to safely seal the drug inside. Once the caps are in place, the nanospheres are "washed" to remove the drug from the outer surface.

Controllable caps

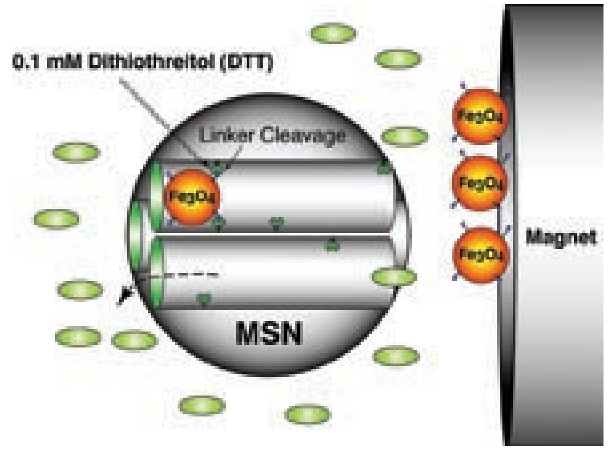
The type of material used for the end caps, how they're held in place and how they're released is the focus of Lin's work. The caps can be dendrimers, biodegradable polymers, genes, proteins, metallic nanoparticles or semiconductor nanocrystals – also known as quantum dots – and are held in place by chemical bonds.

Mesoporous silica nanospheres are the focus of Victor Lin's research

(left) Living human cervical cancer cells containing mesoporous silica nanospheres capped with iron-oxide nanoparticles are drawn through solution toward a small rare-earth magnet placed beside the vial.



This diagram shows how the iron-oxide caps hold the drugs within the channels in the nanospheres.



By manipulating the magnetic field, the caps "pop" free, releasing the drug.

Once the nanospheres are inside the target cells, a trigger is used to pop the caps off and release the drug.

"We're looking at two levels of control," Lin says of the trigger mechanism. "One level is to have the cell control the release and the other would be to control the release externally." Lin explains that the chemical-bond holding the cap in place can be engineered to be unphased by chemicals present in normal cells. However, in cancer cells these chemicals, such as antioxidants, appear in much higher concentrations and would break the bonds on the caps and release the drugs. In this way, only cancer cells could be targeted with powerful chemotherapy drugs, such as Taxol or doxorubicin, while the nanospheres inside the normal cells would remain capped and not cause unwanted side affects by damaging healthy cells.

To achieve external control, Lin is using iron-oxide nanoparticle caps that can be manipulated by a magnetic field. In a simple demonstration of the principle, Lin holds a small rare-earth magnet up to a liquid-filled glass vial containing human cervical cancer cells grown *in vitro* that contain nanospheres capped with iron-oxide particles. The cells slowly migrate and cluster to the side of the vial next to the magnet.

"By using a powerful magnet, we can first concentrate the nanospheres at a particular point, such as a tumor site, and then use the magnetic field to remove the caps and release the drug," Lin says. "The advantage of using a magnetic trigger as opposed to an ultraviolet light trigger is that there's no limit to the depth of tissue we are able to probe – think of an MRI."

Other possibilities

Beyond the possibilities for intercellular drug delivery, the nanospheres may provide the key to studying what takes place within a cell. Currently, scientists have difficulty introducing chemicals or genes into cells without either damaging the cell or causing a chain reaction of events that can't be tracked.

"With current gene therapy, it's possible to switch genes on and off, but you don't really know if you are affecting other parts and processes of the cell as well," Lin says. "You may be able to get a plant cell to produce a certain desired product, but the yield may drop significantly." By using externally controlled nanospheres, Lin explains that it may be possible to sequentially release genes, chemical markers and other materials within cells in order to track what happens and what specific changes take place. This phase of Lin's research ties into a larger plant metabolomics project at Ames Laboratory being undertaken by senior chemist and Chemical and Biological Sciences Program Director, Ed Yeung.

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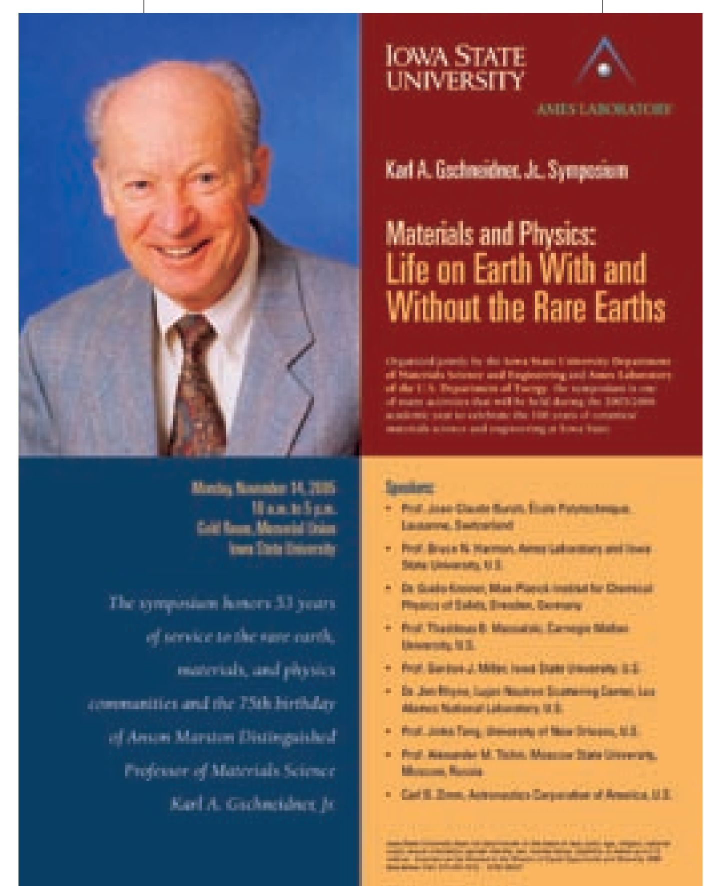
MILESTONES

Symposium honors Ames Lab's "Dr. Rare Earth"

Scientific excellence. Exemplary researcher. Prolific writer. Significant contributor. Colleague, mentor and friend. Wonderful human being! These were just some of the phrases used by speakers and colleagues to describe Ames Laboratory senior metallurgist Karl Gschneidner, Jr. during a symposium bearing his name. The event, held Nov. 14, 2005, honored Gschneidner's 53 years of service to the rare earth, materials and physics communities, and celebrated his 75th birthday.



Entitled "Materials and Physics: Life on Earth With and Without the Rare Earths," the symposium brought some of the top researchers from around the world to share their expertise. Sponsored jointly by Ames Laboratory and the Iowa State University department of materials science and engineering, the event was also one of several activities planned to observe 100 years of ceramics/materials science and engineering at Iowa State.

Ames Lab senior scientist Vitalij Pecharsky, who helped organize the symposium, kicked off the event with a short tribute to his close colleague.

"It's been my privilege to know Karl for the last 16 years," Pecharsky said. "He is one of the finest human beings I have ever known in my life, and it's been a pleasure organizing this symposium. It's a fitting way to recognize what Karl has done, not only for this community, but for scientists throughout this country and around the world."

Ames Lab Director Tom Barton shared a letter from DOE Office of Science Director Ray Orbach, who congratulated Gschneidner on his 53 years of "prolific and dedicated service to the rare earth community. This (symposium) is a most fitting way to acknowledge someone whose expertise is so recognized and respected that the scientific community regards you as 'Mr. Rare Earth.' "

Adding his own congratulations, Barton said, "I'd like to say happy birthday and a very sincere thank you for the tremendous contributions that you have made to the scientific, international reputation of the Ames Laboratory. You've certainly earned the nickname, but I think we ought to at least promote you to 'Dr. Rare Earth.' "

"On a personal note, Karl, your infectious enthusiasm for, and your obvious, genuine enjoyment of, your science has always served as a constant reminder to me that great science is great fun," Barton added.

Reflecting on his symposium, Gschneidner thanked the organizers and the presenters.

"The quality of the presentations was so outstanding, I actually stayed awake through all of them," he said with a characteristic twinkle in his eye.

Chemist John Corbett turns 80

On Thursday, March 23, 2006, Ames Laboratory senior chemist John Corbett turned 80, and the occasion did not go unnoticed by his friends and co-workers at Ames Lab. A birthday celebration, complete with cake, was held to observe the milestone for the man who has been a member of Ames Laboratory's research team for 53 years.

Corbett, who is still actively involved in research, is also an Iowa State University Distinguished Professor of Liberal Arts and Sciences, has served as chair of the chemistry department and as division chief and program director in the Ames Laboratory. He is a Fellow of the American Association for the Advancement of Science. Among his honors are the ACS Awards in Inorganic Chemistry and in Distinguished Service in the Advancement of Inorganic Chemistry, a Senior Scientist Award from the A.V. Humboldt Foundation, two DOE Awards for Outstanding Scientific Accomplishments in Sustained Research in Materials Chemistry, and election to the National Academy of Sciences.

To honor Corbett, Ames Laboratory Director Tom Barton presented the longtime researcher with a plaque bearing the following inscription: "To John Dudley Corbett on the occasion of your 80th birthday, we take the opportunity to thank you for the luster that your scientific achievements have brought upon the Ames Lab and Iowa State University."

"Radical" Means

Researchers solve century-old chemistry conundrum

BY SAREN JOHNSTON

For more than 100 years, chemists debated the nature of the mechanism that triggers the Fenton reaction, one of the most powerful oxidizing reactions available for breaking apart organic compounds. Back and forth the controversy persisted, generating a profusion of professional articles that supported either one or the other of the likely candidates – short-lived, difficult-to-measure hydroxyl radicals or the extremely rare iron(IV). Which one was the highly reactive Fenton intermediate that could initiate the oxidations of countless substances, from biomolecules, such as proteins, sugars, fatty acids and nucleic acids to the pollutants found in smog and industrial wastes?

Decades passed, and the identity of the elusive Fenton intermediate remained a mystery. Now, however, Ames Lab senior chemist Andreja Bakac and assistant chemist Oleg Pestovsky have generated, characterized and ruled out iron(IV) as the Fenton intermediate. Their irrefutable research results tip the balance heavily toward hydroxyl radicals, or OH radicals, as the crucial intermediate by which the Fenton reaction proceeds to completion.

Fenton facts

Discovered in 1894 by H. J. H. Fenton, the Fenton reaction is the oxidation of aqueous iron(II), or Fe(II), with hydrogen peroxide, a versatile, safe and effective oxidant. (An oxidant is a substance containing oxygen that reacts chemically with other materials to produce new substances.)

The pervasive nature of the Fenton reaction accounts for scientists' longstanding efforts to unravel the century-old mystery surrounding the famous Fenton intermediate that allows the reaction to proceed to completion. And no wonder – the reaction operates or is employed almost everywhere, with both good and not-so-good effects. It's critical in the treatment of organic pollutants that are introduced into the environment by the uncontrolled use of such things as pesticides and herbicides, among many other man-made contaminants. It's vital within the industrial chemistry arena, where researchers investigate catalysts with the goal of making various chemical processes go faster and in a more selective and efficient manner. In contrast, the Fenton reaction plays not-so-benign roles in the biology of aging and disease, contributing to certain types of DNA damage that may not self-repair and, so, accumulate with age.

(left) Bakac and Pestovsky bubble ozone through a solution and use it to generate Fe(IV).

Closing in on the chemistry

"Knowing the nature of the intermediate is crucial to understanding the role of Fenton chemistry in issues related to environmental and atmospheric chemistry, as well as human health and aging," says Bakac, who is also an Iowa State University adjunct professor of chemistry. "The fact that we have now eliminated iron(IV) in Fenton reaction and confirmed it in ozone reaction, may provide a foundation for the development of new and useful catalytic reactions based on iron(IV)."

Ames Lab's basic research effort was done in collaboration with Carnegie Mellon University in Pittsburgh and the University of Minnesota in Minneapolis. An article by the collaborating scientists describing their research and its indisputable results was published in *Angewandte Chemie*. The journal gave the article a "Very Important Paper," or VIP, rating, which less than 5 percent of their manuscripts receive.

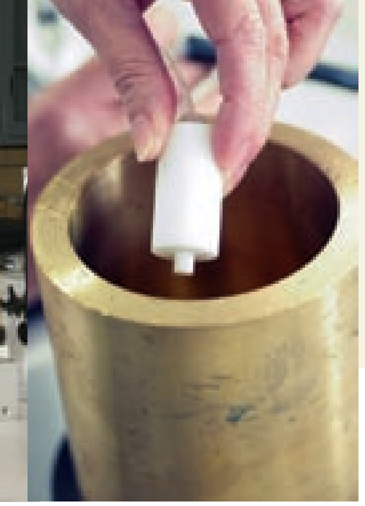
As with many scientific achievements, the work done by Bakac and Pestovsky that eventually ruled out iron(IV) as the Fenton intermediate did not initially have that goal. "We started out studying aqueous iron(IV) for several reasons," says Bakac. "It is a very unusual species, but in stabilizing biological environments, iron(IV) has been found to play a role, especially in enzymatic reactions. And as soon as you find something that is considered unusual to actually function in real life, you know it's not that uncommon – it just hasn't been recognized before."

Andreja's idea

"Iron(IV) was not a totally unknown species when we started looking at it," says Bakac. A research group in Denmark had done the reaction of iron(II) with ozone and proposed that iron(IV) was produced," she explains. "That was about a decade ago, and the work kind of went unnoticed."

While reviewing the literature relating to iron(IV), Bakac came across the Danish papers again. "As I read those papers, I figured if that was iron(IV), then there ought to be much more chemistry there, some of it potentially important in both catalytic and biological contexts," she says. "Of course, nobody knew whether iron(IV) was really involved. It was some sort of intermediate that hadn't been characterized. This is where Oleg and I got involved."

Bakac and Pestovsky set out to generate this species from iron(II) and ozone, and look at its chemistry. "All along we were hoping to find that this really was aqueous iron(IV), a simple, but probably extremely reactive species," Bakac says. "The initial reactivity data were truly exciting and consistent with an iron(IV) species, but still we had no proof," she adds.



*(left) **Preserving a life:** Andreja Bakac demonstrates the device that allows her and Oleg Pestovsky to generate and freeze iron(IV) in less than a second.*

*(right) **Very "cool" stuff:** A delicate spray of newly generated iron(IV) has frozen instantly to the inner walls of this copper cylinder that has been cooled to liquid-nitrogen temperature (77 Kelvin, or minus 321 degrees Fahrenheit).*

Mössbauer "magic"

"We saw some beautiful chemistry, but we definitely needed to identify this species," says Bakac, "so we got in touch with Eckard Münck at Carnegie Mellon. He's the world expert in Mössbauer spectroscopy, which is considered to be the most definite of spectroscopic methods when working with iron."

Bakac explains that iron(IV) is a short-lived species, lasting about 10 seconds at room temperature. Although that is orders of magnitude more than some intermediates she works with that live only milliseconds or microseconds, Bakac notes that the 10-second life of iron(IV) did present a problem. "It was a lot to deal with when we were producing the material here in Ames and the group that was analyzing it was in Pittsburgh," she says. Fortunately, the two research teams collaborated and found a way to get a sample from Ames to Pittsburgh before it "died."

"We designed and built a device that allows us to generate iron(IV) and immediately cool it down to liquid nitrogen temperature and freeze it in a fraction of a second," says Bakac. "We then packed the solid into a liquid-nitrogen-cooled dewar and shipped it overnight to Pittsburgh. There, the Carnegie Mellon team collected the Mössbauer spectrum at liquid helium temperature."

Mössbauer studies of the Ames samples done under Münck's direction by Carnegie Mellon research associate Emile Bominaar and graduate student Sebastian Stoian proved the intermediate generated by Bakac and Pestovsky was exactly what they were hoping for – the iron(IV) species.

In addition to the Carnegie Mellon work, contributions by Lawrence Que and his postdoctoral associate Xiaopeng Shan at the University of Minnesota further confirmed the iron(IV) species. "They took our sample to Stanford University to get an X-ray absorption spectrum, or XAS, and that spectrum was consistent with the oxidation state of iron(IV)," says Bakac.

The Mössbauer and XAS analyses, combined with all the chemistry carried out at Ames Lab, told Bakac and Pestovsky what iron(IV) looks like and what it does. "For the first time we knew what both iron(IV) and OH radicals would do and could figure out which one is involved in the Fenton reaction," says Bakac. "Nobody knew how to make iron(IV) or look at it before so that we could distinguish between the two."

Identical experiments, different products

At that point, knowing the nature of the intermediate, Bakac and Pestovsky decided to carry out some very specific experiments. In one set of experiments, they oxidized a substance with iron(IV), and in a parallel series of experiments, they oxidized the same substance using the Fenton reaction.

"The products were different," says Bakac. "And more than that, the products generated from the Fenton reaction were identical to those known to be formed from reactions involving OH radicals. So we both ruled out iron(IV) as the intermediate and indirectly confirmed OH radicals," she says.

Bakac and Pestovsky's work took about a year, and not every sample was good. "There were times when we thought our samples weren't surviving the trip, so on one occasion Oleg actually traveled to Pittsburgh with all of our equipment to make the sample there," recalls Bakac. "It's been rocky at times, but we knew we had something special, and that kept us going."

In addition to ruling out iron(IV) and indirectly establishing OH radicals as the Fenton intermediate, Bakac and Pestovsky's research shows iron(IV) to be a very useful chemical species. "The fact that iron(IV) is very short-lived doesn't matter because in catalytic reactions you can make it in situ and use it immediately," says Bakac. "There are certainly situations in chemistry and biology where various iron(IV) complexes, including our aqueous iron(IV), may be involved," she suggests, then adds; "just don't go searching for iron(IV) anymore in Fenton chemistry."

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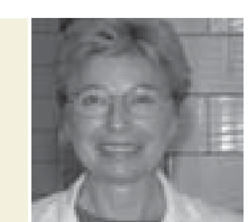
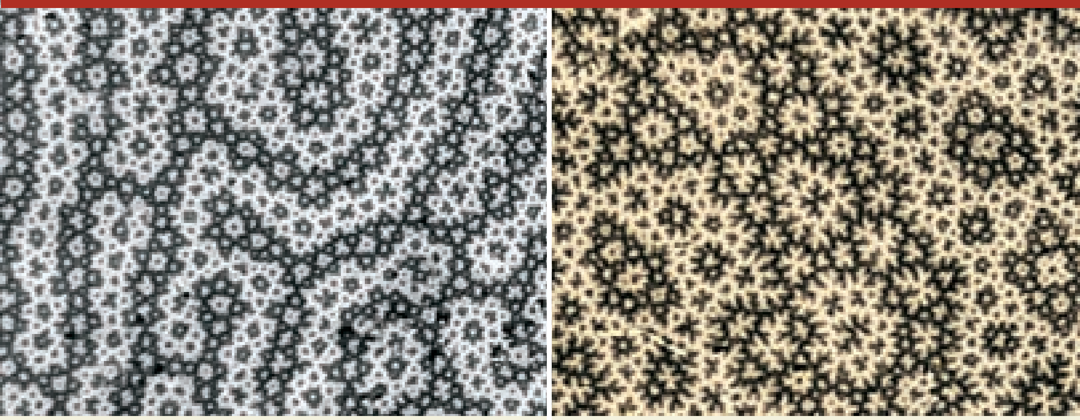
Research funded by:
DOE Office of Basic Energy Sciences, Chemical Sciences Division



Cunning Patterns of Excelling Nature

Shakespeare's *Othello*



Different magnifications of a neodymium-iron-boron single crystal (grown in senior physicist Paul Canfield's lab) show the distribution of magnetic domains. The elaborate patterns provide Ruslan Prozorov with clues to the material's physical properties.

The tunnel diode resonator allows experimental sensitivity far exceeding commercial setups for studying the properties of superconducting materials.

Ruslan Prozorov prepares a sample for low-temperature magneto-optics study. He applies his own unique measurement techniques to analyze the relationship between the patterns created in the presence of a magnetic field and the macroscopic magnetic properties of the material.

From temperatures hovering near absolute zero comes clever, spectacular physics

BY SAREN JOHNSTON

Ruslan Prozorov

RUSLAN PROZOROV adjusts the image on his computer monitor, and a magnificent geometry appears. He's literally seeing the magnetic fields associated with the magnetic moments in the crystalline surface of the material under investigation. Somewhat reminiscent of fractals – objects that display self-similar structure over an extended scale range – the geometries Prozorov sees are complex and detailed. The intricate patterns fascinate him, not only for their beauty, but more importantly for their potential to reveal more about a material's physical properties.

"One of my deep interests in physics is to relate the geometry of the magnetic field patterns to the physical properties of a material," says Prozorov an Ames Laboratory associate scientist and an Iowa State University assistant professor of physics. "There are a wide variety of patterns, and I want to understand their connection to actual, measured physical properties."

Prozorov says textbooks often ignore the intricacy of the magnetic field patterns. "Nature behaves in a much more complex way than textbooks tend to describe," he emphasizes. And for Prozorov, that complexity is best studied at the extremely low temperatures associated with liquid helium – around 4.2 Kelvin, or minus 452.11 degrees Fahrenheit – just a few degrees above absolute zero. At these extremely cold temperatures, materials are almost completely free of excitations and vibrations, making it possible to create magnetically ordered or superconducting states – the subjects of Prozorov's investigations.

Magneto-optics "magic"

To shed light on the physical properties of a material, Prozorov employs magneto-optics, a tool that allows him to study the effects arising from the interaction of light with magnetized media. By applying his own unique experimental techniques, he makes the most of what magneto-optics has to offer.

"One of the key ingredients is that I'm able to reach a wide range of temperatures. I can pass liquid helium through the system and observe a material at a few degrees above absolute zero," he says. Taking advantage of the magneto-optical Faraday and Kerr effects, which account for the rotation of the plane of polarization in a magnetic field, Prozorov can observe how the magnetic field patterns form and explore the connection between those patterns and the material's physical properties. "I can literally see the magnetic field with my own eyes," he says.

Prozorov explains that magnetism comes from electrons and their interactions, and each electron has a magnetic moment associated with it called spin. "Spin is actually a mechanical concept, but it's used to refer to the magnetic moment of an electron," he says. In magnetic materials, the magnetic moments can be aligned either up (spin up) or down (spin down). "That's exactly what we're seeing with the magneto-optics," he continues. "Spin up corresponds to bright intensities in the patterns, and spin down corresponds to darker intensities." He notes that these regions of "ups" and "downs" might seem fairly basic, but the reality is much more complex, involving structures of different length scales that are quite fractal in a sense.

Describing his research on magnetism at low temperatures, Prozorov says it is both fundamental and applied. He notes that the fundamental aspect revolves around the use of new tools, such as his magneto-optical setup, to study and measure the physical properties of materials. It's also applied research because unless you know how a material behaves on a small scale, you don't know if it will behave the way you expect it to in a real application. "Part of the reason for a material's unexpected behavior may be these complex patterns, which, if you understand them, may allow you to apply them to different things," he explains.

Low-temp lab

The magneto-optics system combined with the unique experimental techniques Prozorov brings to it is a mainstay of the new low-temperature lab that he has established in one short year since coming to Ames Laboratory from the University of South Carolina. But it is not the only one. A state-of-the-art dilution refrigerator capable of reaching temperatures as low as seven thousandths of a Kelvin above absolute zero provides an unimaginably cold environment in which Prozorov can apply his innovative methods to study various materials and discover more about their physical properties.

Perhaps one of Prozorov's most outstanding contributions to the burgeoning low-temperature lab is the tunnel diode resonator. The device, which is not available commercially, is a self-resonating circuit that is extremely stable and provides experimental sensitivity exceeding commercial setups by orders of magnitude. Prozorov uses it to study properties of superconducting materials.

"There are only a few similar systems in the United States and Europe, and that's it," says Prozorov.

"Cool" work brings recognition

Prozorov's exceptional work on magnetism and superconductivity at low temperatures has not gone unnoticed. He was selected as one of only 23 scientists in the United States to receive a 2006 Sloan Research Fellowship in physics. The prestigious awards are intended to enhance the careers of bright young faculty members in specified fields of science. In addition to the prominence it affords the recipients, the Sloan Research Fellowship provides a cash reward. Prozorov will receive $45,000 over a two-year period, which he may use to support any activity directly related to his research.

As he considers how he wants to apply the funds he'll receive from the Sloan Research Fellowship, Prozorov says he feels fortunate to be a member of the Ames Laboratory research community. "Ames Lab is a unique place in terms of magnetic and superconducting materials, and that's a key ingredient for me," he says. "I don't generally make materials, but I know how to measure them," he adds with aplomb.

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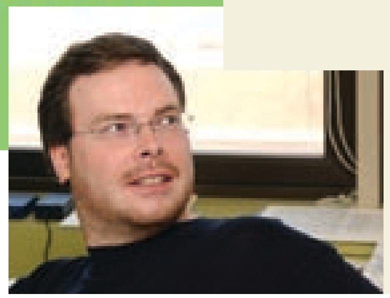
Fast Backward Motion

Metamaterials put a new slant on light – it's direction and speed

BY SAREN JOHNSTON

Negatively refracted light.



Thomas Koschny

LIGHT FLIES. IT ZIPS BY, MOVING EVER FORWARD at a mind-boggling 186,000 miles per second, the speed at which electromagnetic waves can move in a vacuum. That, folks, is "flying!" And Ames Laboratory senior physicist Costas Soukoulis and his research team are getting in on the action.

They're having the times of their lives reversing light's "flight pattern," making it travel backward at negative speeds that appear faster than the speed of light. The whole process is what Soukoulis, who is also an Iowa State University Distinguished Professor of physics and astronomy, says is "like rewriting electromagnetism." He predicts, "Snell's law on the refraction of light is going to be different; a number of other laws will be different."

Costas Soukoulis

Marvelous metamaterials

There's no stopping light as it zips along on the fast track to anywhere and everywhere it pleases. However, there is control. Researchers can manipulate light by using exotic, artificially created materials. Known as metamaterials, these substances can be created to respond to electromagnetic waves in ways that natural materials cannot. Natural materials refract light, or electromagnetic radiation, to the right of the incident beam at different angles and speeds. (An incident beam is one that strikes a surface.) However, metamaterials, also called left-handed materials, make it possible to refract light at a negative angle, so it emerges on the left side of the incident beam. This backward-bending characteristic of metamaterials allows enhanced resolution in optical lenses, which could potentially lead to the development of a flat superlens with the power to see inside a human cell and diagnose disease in a baby still in the womb.

Whittling down the wavelength

The challenge that Soukoulis and other scientists who work with metamaterials face is to fabricate them so that they refract light negatively at ever smaller wavelengths, with the ultimate goal of making a metamaterial that refracts light at visible wavelengths and achieving the much-sought-after superlens. Admittedly, that goal is a ways off. To date, existing metamaterials operate in the microwave or far infrared regions of the electromagnetic spectrum. The near infrared region of the spectrum still lies between the microwave and visible regions, and the wavelengths become ever shorter moving along the electromagnetic spectrum to visible light. Correspondingly, to negatively refract light at these shorter wavelengths requires fabricating metamaterials at extremely small length scales – a tricky feat.

However, recent research by Soukoulis and his co-workers from the University of Karlsruhe, Germany, published in the May 12, 2006, issue of *Science* demonstrates they have done just that. "We have fabricated for the first time a metamaterial that has a negative index of refraction at 1.5 micrometers," says Soukoulis. "This is the smallest wavelength obtained so far." Small, indeed; these wavelengths are microscopic and can be used in telecommunications. Soukoulis' success moves metamaterials into the near infrared region of the electromagnetic spectrum – very close to visible light, which would permit superior resolution and a wealth of potential applications.

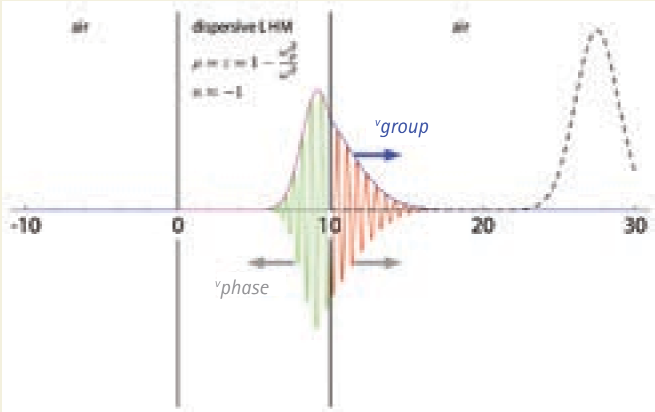


Fig. 1: Realistic metamaterial with dispersion – A wave packet strikes a physical, dispersive metamaterial slab from the left and then travels to the second interface of the slab. The group velocity (that of the wave packet) is positive both inside and outside the slab. The phase velocity (that of the individual wavelengths) is negative inside the slab. There is no violation of Einstein's theory of relativity. The dashed line represents the predicted position of the wave packet if the metamaterial slab had not been there.

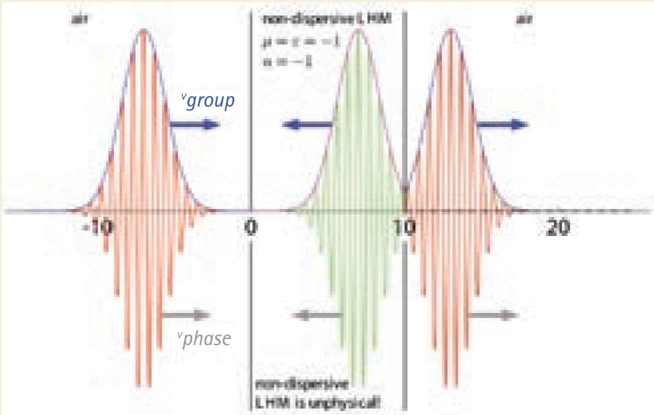


Fig. 2: Fictitious (theoretical) metamaterial without dispersion — The same situation as in Fig. 1 is shown for an unphysical, dispersionless metamaterial. A wave packet strikes the first interface of a nondispersive metamaterial slab from the left. While the wave packet is still outside the slab, a response is already forming at the second interface of the metamaterial. A wave packet is generated and leaves the slab to the right while a second packet is sent backwards through the slab (with negative phase and group velocities) and will eventually annihilate the original wave packet at the first interface of the slab. This situation violates special relativity. Thus, the assumption of no dispersion in metamaterials is fictitious (unphysical).

Revealing experiments

Not only did Soukoulis and his University of Karlsruhe colleagues bring metamaterials closer to visible light, the work yielded something unexpected. The researchers transmitted a laser pulse through a fictitious (theoretical), nondispersive metamaterial (one that does not spread out the light pulse into individual wave components with different velocities). The experiment showed that the velocity of the individual wavelengths, called phase velocity, was negative inside the metamaterial. In addition, the experiment showed, contrary to popular thought, that the velocity of the wave packets, called group velocity, can also be negative simultaneously.

"We can have a wave packet hit a slab of negative index material, appear on the right-hand side of the material and begin to flow backward before the original pulse enters the negative index medium," says Soukoulis. "This is possible because the components of the wave packet can be reshaped and make a pulse inside the dispersion medium before the original pulse enters the negative index medium. In this way, one can argue that the wave packet travels backward with velocities much higher than the velocities of light, seemingly defying Einstein's theory of relativity," he says.

In experiments with a more realistic metamaterial with dispersion, the researchers found that the phase velocity can be either positive or negative, depending on the frequencies of the dispersed light being studied. "When we have a metamaterial with a negative index of refraction at 1.5 micrometers with dispersion, we can tune our lasers to play a lot of games with light," says Soukoulis. "This is due to the dispersion of the negative index of refraction; there is nothing wrong with Einstein's theory of relativity."

Making movies

The detailed interactions of electromagnetic radiation within metamaterials lead to phenomena that are counter-intuitive and difficult to explain in ordinary terms. To help clarify the out-of-the-ordinary nature of the experimental results obtained by Soukoulis and his University of Karlsruhe collaborators, postdoctoral fellow Thomas Koschny has taken on the additional role of metamaterial movie-maker for the research team. He has developed simulations that depict a pulse of light entering both a fictitious metamaterial without dispersion and a realistic metamaterial with dispersion. So if like most of us you find the relationship between electromagnetism and metamaterials a difficult one to understand, grab your popcorn and soda and go check out the movies at: *www.external.ameslab.gov/final/News/Lightmovies.htm.*

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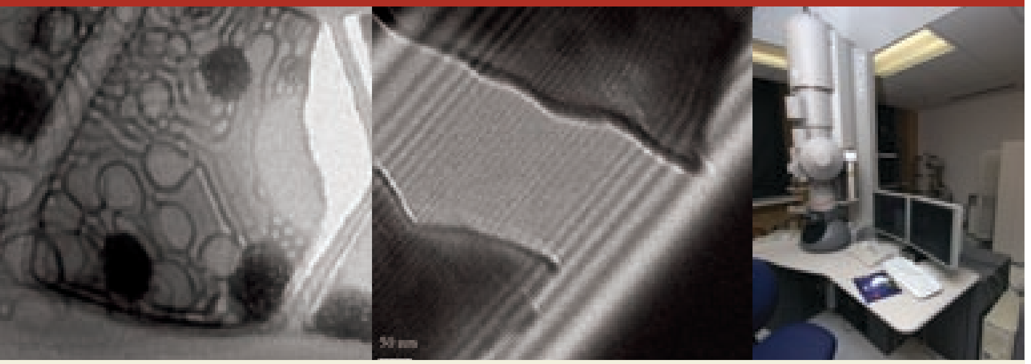
DOE Office of Basic Energy Sciences,
Materials Science and Engineering Division

New Window on the Nano World



Viewing polymer films (left) and magnetic fields in materials are just two capabilities now available with the new FEI-Tecnai G2 - F20 scanning transmission electron microscope recently installed in Ames Laboratory's Wilhelm Hall. The $1.8 million microscope not only offers high resolution, but takes researchers only a fraction of the time to focus and capture digital images.

New $1.8 million scanning transmission electron microscope

BY KERRY GIBSON

RESEARCHERS AT AMES Laboratory can now see the atomic structure of materials with unprecedented clarity thanks to a new $1.8 million scanning transmission electron microscope. The new FEI-Tecnai G2 – F20 STEM was installed in Wilhelm Hall this summer.

A transmission electron microscope uses high-voltage electron beams to acquire ultrahigh resolution sample images down to Ångström levels for analyzing the atomic structure, crystallographic structure and composition of specimens. The specimens are typically thinned through ion milling or other techniques to a film only a few nanometers thick so that the beam can pass through the sample.

The entire electron path, from gun to screen, must be under vacuum (otherwise the electrons would collide with air molecules and be absorbed), so the final image has to be viewed through a window in the projection chamber. Unlike a light microscope with glass lenses, the electron beam is focused using electromagnetic lenses. By varying the current through the lens coil, the focal length, which determines the magnification, can be varied.

The scanning function employs electron optics to focus the beam into a narrow spot. The beam is scanned back and forth over the sample to form an image.

According to Ames Lab scientist Matt Kramer, who is overseeing the operation of the STEM, the new scope will provide much more than just higher resolution than the existing Phillips CM30 STEM.

"One of the big differences is in the scanning probe size," Kramer says. "While the CM30 in theory could do a 1.2 nanometer probe, it had no brightness at that fine probe size. The new STEM has a probe of 0.18 nm with more than a factor of 100 times more brightness." This will allow for very precise measurements of chemical changes over a few nanometers.

The new machine also has computerized alignment and focusing, which dramatically reduce set-up time. Individual users can even save specific settings and call them up at a later date if they want to look at additional samples.

"The old equipment often required hours to align and focus the beam — it was really an art," Kramer says. "The new equipment is automated so each user can save specific settings, and the computer will realign the beam to those settings in a matter of seconds."

Another big difference is the image capture. The older machine uses photographic plates to record images, while the new microscope captures digital images that can be displayed immediately.

While the new machine can perform standard operations, such as bright field, dark field and lattice imaging, it also has features that allow energy-filtered imaging, low-dose imaging, Lorentz imaging, holographic imaging, Z-contrast imaging and 3-D imaging.

"The low-dose imaging is useful when working with sensitive materials, such as polymer films, that could be damaged by the beam," Kramer says. "You can focus the beam on areas outside the main area of interest, then quickly move to the region you want to look at. The older equipment doesn't allow this. By the time you get it focused, the beam has disrupted the structure of the sample."

The Lorentz lenses, coupled with the holographic feature, allows vivid depiction of features such as magnetic fields. And a tomography stage allows the sample to be rotated through various views, which are then assembled into a 3-D image.

With all these capabilities, the equipment is understandably complicated, so not just anyone will have access to it. This means long-term collaborative projects will be given preference along with projects funded by the Office of Basic Energy Sciences. BES provided the funding for the equipment through a special grant in 2005.

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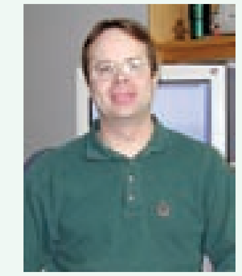
2005-2006 AWARDS

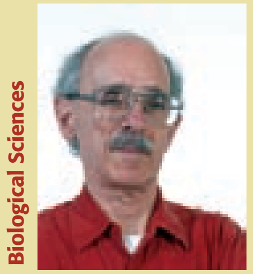
Applied Mathematics and Computational Sciences

Mark Gordon
- ISU Award for Research or Artistic Creativity
- ISU Master Teacher Award



Brett Bode
- IBM Faculty Award. "Management and Control Software for Peta-Scale Systems"

Chemical and Biological Sciences

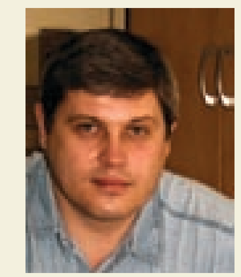


Mark Gordon
- ISU Frances M. Craig Chair Professorship

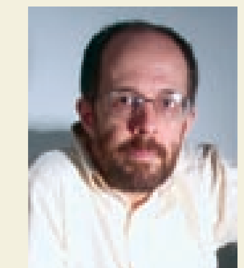
Edward S. Yeung
- Martin J. Golay Medal
- Merit Award, Chicago Chromatography Discussion Group

Condensed Matter Physics

Costas Soukoulis
- DesCartes Prize (see page 9)
- ISU Distinguished Professor

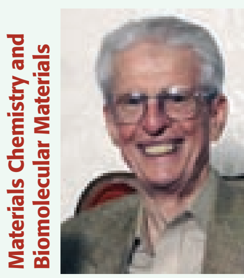


Ruslan Prozorov
- Sloan Research Fellowship

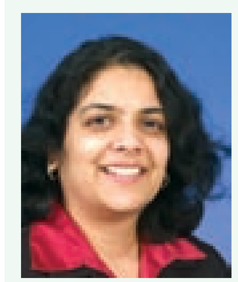


Paul Canfield
- ISU Distinguished Professor

Materials Chemistry and Biomolecular Materials

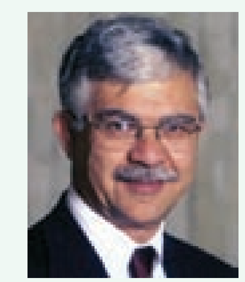


John D. Corbett
- F.H. Spedding Award in Rare Earth Research



Surya K. Mallapragada
- Fellow, American Institute of Medical and Biological Engineering

Dan Schectman
- Honorary member, Japan Institute of Metals



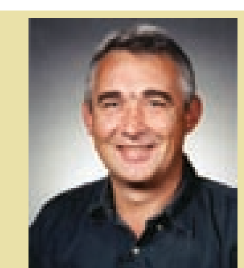
Mufit Akinc
- Ross Coffin Purdy Award, American Ceramic Society

Cynthia Jenks
- ISU Professional and Scientific CYtation Award
- Board of Regents Staff Excellence Award

Patricia A. Thiel
- Dr. Honoris Causa, Institut National Polytechnic de Lorraine

Materials and Engineering Physics

Brian Gleeson
- ISU Alan and Julie Renken Professor in Materials Science and Engineering



Vitalij K. Pecharsky
- ISU Anson Marston Distinguished Professor of Engineering

Karl A. Gschneidner, Jr.
- ISU Materials Science and Engineering Excellence in Research Award

Ames Laboratory's education programs this year spanned the range from elementary school students to undergraduates, through tours and science night activities, Middle School and High School Regional Science Bowls and the Science Undergraduate Laboratory Internship program. And steps are underway to extend that even further, bringing middle teachers into the laboratory setting for an intensive science education experience.

For the 16th straight year, teams of high school students from across Iowa traveled to Ames the last weekend in January to participate in the Ames Laboratory/ISU Regional High School Science Bowl. After losing an early match to defending champion Ames High School, Iowa City Regina advanced to the finals and defeated Ames twice to win the 2006 championship and advance to the National Science Bowl.

At the national competition, the Regina team of Phil Shiu, Peter Montag, Josh Hove and Stephen Berg made a strong showing, placing in the "Sweet 16" teams and winning $1,000 for the school.

"I'm so proud of these students," said Regina coach Barb Reilly. "It's amazing that a school our size (less than 300 high school students) was able to get to this level." In comparison, Miami Palmetto High School, which eliminated Regina from competition, had 3,400 students. Reilly said the Regina team will consider using their winnings to purchase a mini library of information and review items that will help future teams prepare for Science Bowl, or they may outfit a lab or buy a microscope.

Evans Middle School of Ottumwa, winner of the Ames Lab/ISU Regional, also finished in the money at the 2006 National Middle School Science Bowl, held June 21-24 in Denver, Colo. The Evans team of Estefany Garcia, Andrew Kaake, Samantha Robertson, Jake Swanson and Jacqueline Vonderhaar finished fourth in the 25-team middle school competition, winning $500 for their school. Evans advanced to the national competition by defeating Boone Middle School in the Ames Laboratory/ISU regional championship on April 8.

(above) A team of middle schoolers assembles a hydrogen fuel-cell car during the opening day of competition.

(below) High school students from Clay Central-Everly confer on a bonus question during the Ames Lab/ISU High School Science Bowl competition.

Year two for SULI

A new group of 10 aspiring scientists participated in the second year of Ames Lab's Science Undergraduate Laboratory Internship or SULI, program. Funded by the Department of Energy's Office of Science, the program focuses on providing internships in real-world research settings at DOE national laboratories to students interested in careers in science and engineering.

Year two of SULI had students working with their Ames Lab/ISU mentors for a 10-week period – two weeks longer than the 2005 inaugural program — to give participants more time to complete research projects and write papers. This year's program began May 30 and continued through August 4.

One of DOE's objectives for the SULI program is to encourage participation by students whose home institutions do not have major research facilities. To help achieve that objective, DOE asks its national labs to make the internships available to students who aren't attending universities in their own backyards. This year's SULI students were all from out of state. Universities and colleges represented included Pennsylvania State University; Western Illinois University; Moraine Valley Community College (Illinois); Ohio State University; Michigan Technological University; BYU, Idaho; Westminster College (Missouri); University of Kansas, Lawrence; Colorado School of Mines; and Carnegie Mellon University (Pennsylvania).

(above) SULI student DeAnna Jones, BYU, Idaho, performs research on the synthesis of magnetic nanoparticles. She worked with mentor Surya Mallapragada and research associate Tanya Prozorov.

(below) Ryan Glamm, SULI student from Ohio State University, studies the crystallography of fractured metal surfaces. He worked with mentors Barbara and Tom Lograsso.

Teaching teachers

In addition to undergraduate students, Ames Lab will begin a program to bring middle school teachers into the laboratory setting for an intensive science-education experience. Called Laboratory Science Teacher Professional Development, or LSTPD, the program will bring 10 teachers from middle schools from Iowa, Minnesota and South Dakota to Ames Lab and ISU to participate in the Teachers as Investigators program. Through the program, teachers will learn how to bring exciting breakthroughs and frontiers of science into their classrooms, while conducting hands-on, discovery-based experiments with advanced equipment.

In coordinating the LSTPD program, Ames Laboratory joins a nationwide effort on the part of DOE's national laboratories in inspiring, educating and encouraging a new generation of scientists who will be equipped to "enhance the science literacy of the nation." This initiative is in keeping with the recommendations of the Secretary of Energy Advisory Board's Science and Mathematics Education Task Force, which recognize the role teachers, especially middle school teachers, play in "maintaining students' enthusiasm for science." The proposed program will require a four-week commitment from teachers each summer for three years.

INQUIRY | 2006

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AMES LABORATORY

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