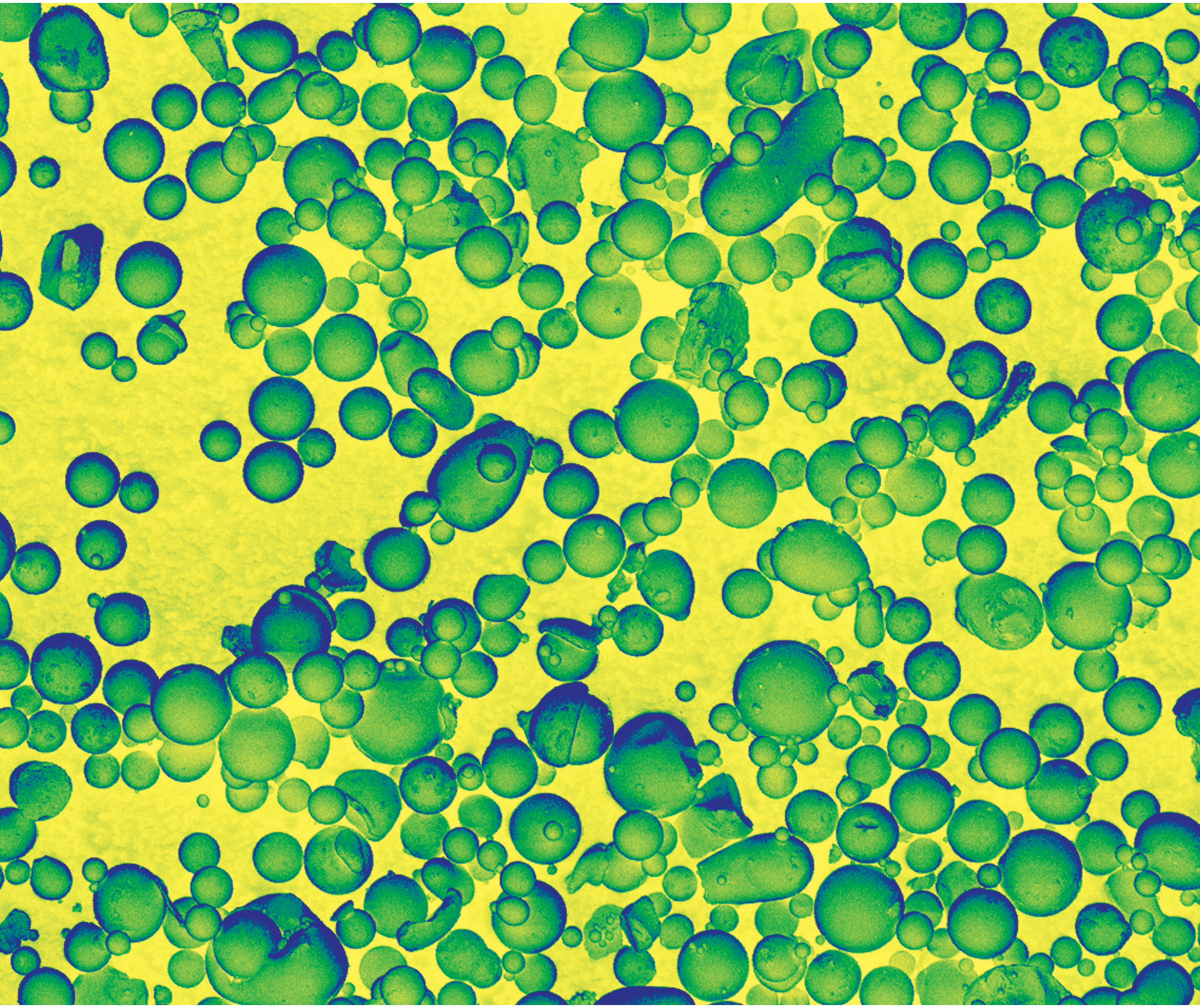
INQUIRY | SPRING 2008

SCIENCE & TECHNOLOGY AT THE AMES LABORATORY



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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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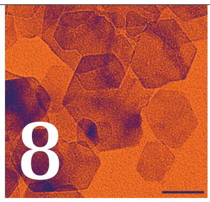
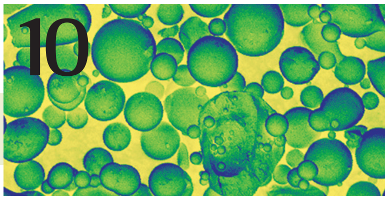




DEPARTMENTS

Cover: *These fine, spherical 2-14-1 permanent magnet alloy powders produced by argon gas atomization may lead to more efficient and economical electric drive motors for ultragreen vehicles.*

From the Director

Let me introduce myself. I'm the new Director of the Ames Laboratory. I arrived in Ames at the beginning of the year after spending eight years at Purdue University, where I was the Head of the School of Materials Engineering. It has been a tough winter in the Midwest, and the burgeoning signs of spring are even more than usually welcome, but the welcome in Ames has been warm at every level throughout the winter.

I am spending some time during my first months here getting to know the Lab and its staff, and I am very pleased with what is emerging. There is certainly a good dose of "Midwestern modesty" here, and a lot of the work is undersold, but I am finding exciting research and exceptional scientific quality in every corner of the Lab. The more people I talk to, the more great science I find.

Ames Laboratory has a great working climate and a rich collaborative environment in which novel ideas are conceived in fundamental science, tested in theoretical and modeling studies, formed into actual materials that you can hold in your hand, and then measured with high sophistication to prove the original concept.

Welcome to the spring 2008 issue of Inquiry *magazine.*

You cannot easily find all of those things working together as well as they do at Ames Lab.

As DOE's Office of Basic Energy Sciences came forth with a new set of "scientific grand challenges" for the research community earlier this year, we were pleased to find that the Ames Laboratory was already working on meeting all of them, and in many cases already has great examples to show.

Energy is grabbing the headlines more than it has since the 1970s as gasoline prices keep rising. More and more often we find ourselves challenged to explain how a Department of Energy lab with a large Basic Energy Science commitment is contributing to meeting the obvious needs. Within these pages, you'll find examples of cutting-edge research that has real potential to provide energy solutions for tomorrow – work that is both fundamental and long-term, but has outcomes that enable energy production with lower environmental impact or consumption with greater efficiency. There is no single "fix" for our energy needs, and there is certainly no quick fix. The energy needs of the future will surely be met through a wide variety of different technologies, all of which will emerge from fundamental scientific research of the kind going on at the Ames Laboratory and its sister labs in the DOE complex. History shows how new technologies most often emerge from new materials, and Ames Lab specializes in designing and inventing materials with novel properties.

I'm excited about the science being done at the Ames Laboratory and about the potential it has to contribute to our energy future and our economic security. Read on for some fascinating examples.

Alex King, Director

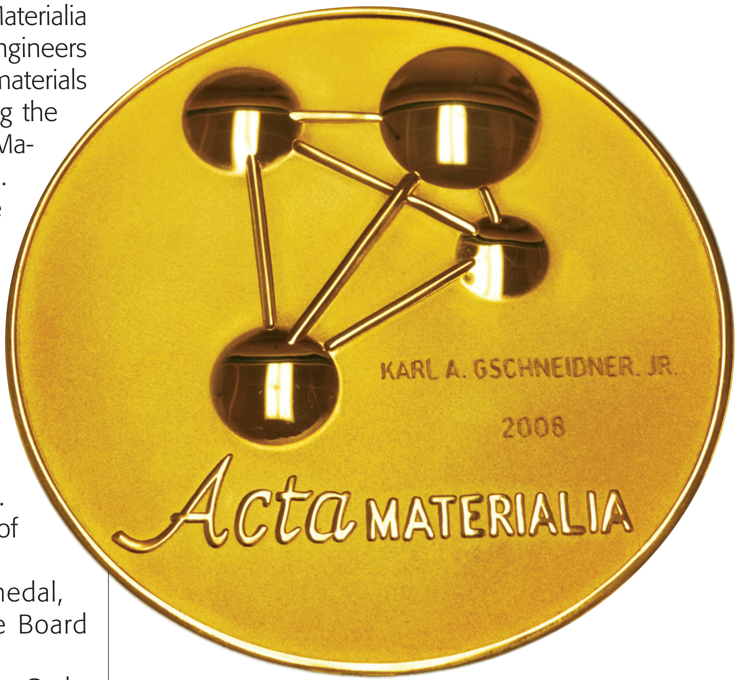
Gschneidner Acta Materialia Gold Medalist

Karl A. Gschneidner Jr., senior metallurgist at Ames Laboratory, has been awarded the prestigious Acta Materialia Gold Medal, considered by many scientists and engineers to be the top award worldwide in the field of materials research. Gschneidner received the award during the 2008 annual meeting of The Minerals, Metals & Materials Society in New Orleans on March 11, 2008.

The Acta Materialia Gold Medal is just the latest of many honors for Gschneidner, who in 2007 was elected to the National Academy of Engineering. The Gold Medal is awarded annually by the Board of Governors of Acta Materialia Inc. with partial financial support from Elsevier Ltd. Nominees are solicited each year from the Cooperating Societies and Sponsoring Societies of Acta Materialia Inc. based on demonstrated ability and leadership in materials research. The candidates are placed on a ballot for a panel of international judges who select the winner.

The award consists of an 18-karat gold medal, an inscribed certificate and a check from the Board of Governors.

The conference also featured a symposium in Gschneidner's honor, with the gold medalist delivering the keynote address.



Karl A. Gschneidner, Jr.

Thompson Wins Excellence Award

R. Bruce Thompson, director of the Nondestructive Evaluation program at Ames Laboratory, has won the Sustained Excellence Award from the American Society for Nondestructive Testing's Research Council.

Thompson, who is also director of Iowa State University's Center for Nondestructive Evaluation and a Distinguished Professor of materials science and engineering and aerospace engineering and engineering mechanics at Iowa State, was nominated by Kevin Smith of Pratt & Whitney. Smith cited Thompson's sustained excellence in research in the field of nondestructive testing through a long career filled with achievements leading to significant advancements in the state of the art.

Bruce Thompson

In addition to Thompson's research achievements, mentoring of students and excellent academic credentials, he was also recognized for his exceptional capability to perceive the possibilities for how theoretical concepts can be applied to industrial concerns.

Anderson TMS Distinguished Scientist/Engineer

Iver Anderson, senior metallurgist at Ames Laboratory, received the 2007 Distinguished Scientist/Engineer Award from the Electronic, Magnetic & Photonic Materials Division of The Minerals, Metals & Materials Society during the society's annual meeting, March 11, 2008 in New Orleans.

Anderson is only the second person selected for the award, which is presented based on a lengthy nomination and peer-review process. Anderson was singled out for his development of a tin-silver-copper solder alloy that has been widely adopted by the electronics industry to remove harmful lead from the environment.

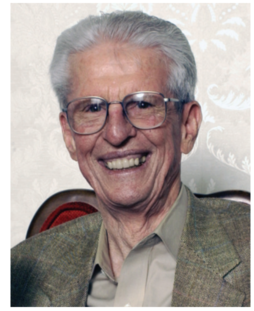
Iver Anderson (left) receives his award from Patrice Turchi, director of the Electronics, Magnetics, & Photonic Materials Division of TMS.

To date, the patented lead-free solder has been licensed by some 60 companies worldwide and has generated nearly $19 million in royalties for Ames Lab and Iowa State University.

The award cites Anderson "for his innovative ideas, his excellent research, his continuing scholarship and the influence he has had on the transition to Pb-free manufacturing."

Corbett Named 2008 ACS Cotton Award Winner

John Corbett, a senior chemist at Ames Laboratory, has been selected to receive the American Chemical Society's 2008 F. Albert Cotton Award in Synthetic Inorganic Chemistry. Established in 2002, the $5,000 award recognizes individuals who have distinguished themselves by demonstrating creativity, imagination and outstanding synthetic accomplishments in the field of inorganic chemistry. The Cotton Award is funded by the F. Albert Cotton Endowment Fund, supported by the late F. Albert Cotton, one of the world's foremost inorganic chemists. Corbett is the fifth recipient of the award.



John Corbett

With his selection for the Cotton Award, Corbett has now received all three awards in inorganic chemistry given by the American Chemical Society. The first was in 1986, when he received the ACS Inorganic Chemistry Award. Then, in 2000, he received the ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry.

Corbett, who is also an ISU Distinguished Professor of Liberal Arts and Sciences and a professor of chemistry, is a member of the National Academy of Sciences.

His research interests lie within the more specialized field of synthetic inorganic solid-state chemistry, which he says has historically been the "forgotten child" of inorganic chemistry.

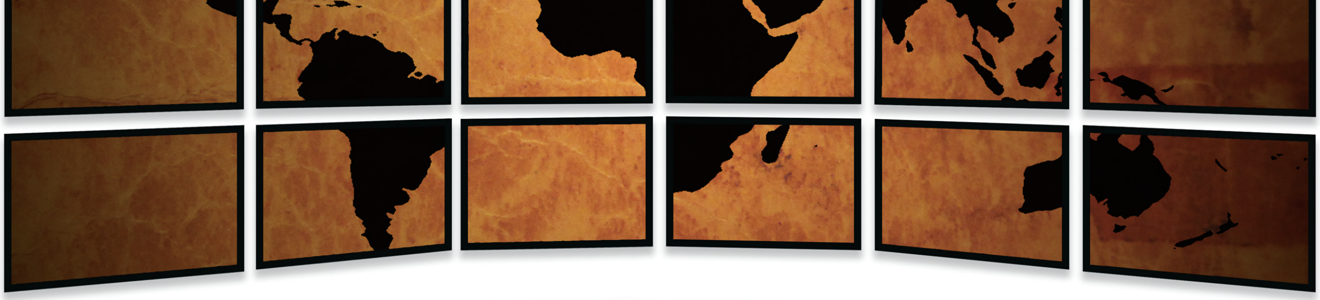
Corbett received the Cotton Award at the 2008 ACS spring meeting in April in New Orleans, where he presented an award address on his research in inorganic solid-state chemistry, including his investigations into strong metal-metal bonding. A symposium in Corbett's honor followed the award address and included many of his former students and postdoctoral associates.

MFRC a Partner in Forensic Technology Center of Excellence

The Midwest Forensics Resource Center at Ames Laboratory is a partner in the newly formed Forensic Technology Center of Excellence that will be headquartered at the National Forensic Science Technology Center located at the Young-Rainey STAR center in Largo, Fla.

The competitively awarded cooperative agreement is the result of the combined efforts of the five partners making up the Forensic Technology Center of Excellence who successfully submitted the peer-reviewed proposal. In addition to the NFSTC and the MFRC, the Center's partners include: Stetson College of Law's National Clearinghouse for Science, Technology and the Law, Gulfport, Fla; the University of Central Florida's National Center for Forensic Science, Orlando, Fla.; and Marshall University's Forensic Science Center, Huntington, W. Va. Each partner is responsible for a specific project in support of the center's objectives.

As a partner, the MFRC will receive approximately $500,000 to support two projects. The first project will target the effective use of process-mapping tools for process improvement, and the second will identify, recruit and retain crime laboratories' scientific staff.



Around the World and Back Again

Former SULI intern returns to Ames Lab

BY STEVE KARSJEN

IT'S NOT TRUE THAT "YOU CAN'T GO HOME AGAIN." Just ask Travis Monk, whose journey back to the Ames Laboratory involved a couple of years, the completion of two degrees and a stay in a foreign country. But in the end, at least temporarily, he came home again to the Lab, conducting interesting and important research.

Monk was an undergraduate at Truman State University when he arrived at Ames Lab for the first time in May 2005. He was one of 10 student interns who participated in the Lab's Science Undergraduate Laboratory Internship, or SULI, program. During his 10-week summer internship, he worked in physicist Kai-Ming Ho's group where his job was to fabricate photonic crystals.


Travis Monk with Kai-Ming Ho

"It turned out that he (Monk) was really among the good people we had for undergraduate interns," says Ho. "We quickly added him to our active recruit list for graduate school at Iowa State."

But graduate school at ISU was not in the cards for Monk upon completion of his undergraduate degree at Truman State in May 2006. Instead, a master's degree in neuroscience rather than physics led him thousands of miles away from the Midwest. His destination: the University of Plymouth in Plymouth, England. In September 2007, following one year of intensive study and completion of his thesis, he graduated from the University of Plymouth with a master's in neuroscience.

Upon receiving his master's degree, Monk once again found himself making decisions about his future. This time, he had to decide where to complete his Ph.D. In the end, he was accepted into the neuroscience program at the University of Otago, Dunedin, New Zealand, but there was one hitch — he couldn't begin until June 2008.

"I had some downtime and I needed a job," says Monk. "So I contacted Dr. Ho with whom I'd worked in 2005. I told him I needed a couple of months of internship, and I was interested in working for him. He offered me a job."

On Oct. 6, 2007, Monk found himself right back at the Ames Lab in an internship involving work on a project similar to the one he'd worked on in 2005.

"I basically did the same work that I did in 2005, fabricating crystals, but this time focused on one particular application for photonic crystals, which is using them as a substance-identification device," he says.

Monk credits the SULI program with providing him the framework to succeed. "I believe it's because I demonstrated to Dr. Ho that I could do good work while I was in the SULI program that he was so willing to offer me a job when I asked," says Monk.

But that's not the only reason Monk spoke so highly about SULI. The program also provided him an opportunity to really figure out what he wanted to do.

"When I arrived at the Lab in 2005, I thought I had my career path laid out. I was interested in theoretical physics, came here and did a project in experimental physics with Dr. Ho, and my career path changed," Monk says. "I'm living proof that the SULI program really helps."

SULI really helps scientists too, says Ho, who credits the program with introducing him to a student he's been able to bring back to the Lab to help perform cutting-edge research in his program. And although things did not quite work out as he'd hoped in that Monk did not decide to come to ISU for graduate school, he says the SULI program served its "global" purpose, which is to get students like Monk to see the value in attending graduate school.

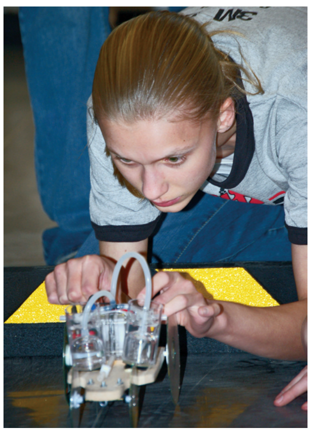
"It's a way for students to see what real research looks like," says Ho. "But also it's a way for scientists to show students how much fun it is being a graduate student and for us to have a channel to reach top students."

Monk's opportunity at Ames Lab lasted only a few months before he was off to New Zealand and the next leg of his education journey. But Ho and the SULI program's investment in him is something that will likely resonate with Monk his entire career. Is there a chance that Monk might find his way back to Ames Laboratory again some day? Quoting Monk, "If neuroscience doesn't work out, I can always go back to physics."

Science Bowl Tradition

High School marks 18th year, Middle School turns five

Ames Laboratory carried on its education tradition hosting the 18th annual High School Science Bowl and the fifth annual Middle School Science Bowl in 2008. Powered by student and staff volunteers from the Lab and Iowa State University, the high school event drew 48 teams from across Iowa on January 26. In April, 16 teams of middle school



Ready, set, GO!

students competed in a two-day event, racing hydrogen fuel-cell cars on Friday, April 18, and then answering science and math questions on Saturday, April 19.

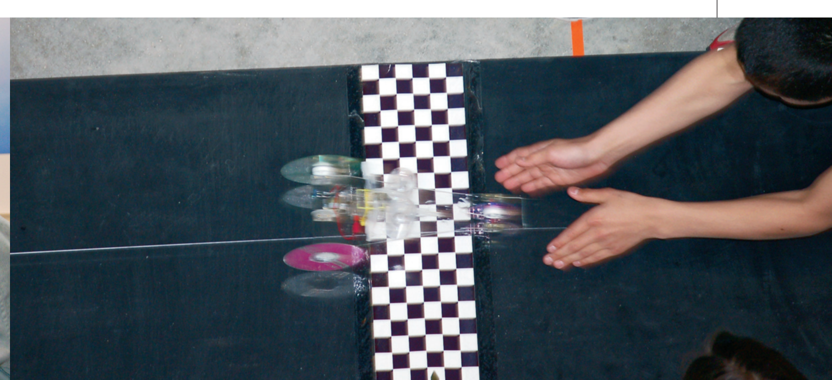
Cedar Rapids-Marion Home Schools won the high school event in only its second year of competition. The team, comprised of seniors Leif Gaebler and Edward Talmage, juniors Evan Gaebler and Andrew Baskerville and freshman Alan Talmage, had a perfect record for the day. They won all five round-robin matches in the morning and defeated West Des Moines Valley, Ames, Home Schools of Eastern Iowa and Des Moines Central Academy on their way to the championship match. Cedar Rapids-Marion was coached by Sally Gaebler and represented the Ames Lab/ISU Regional in the National Science Bowl® May 1-6 in Washington, D.C.

ISU's Howe Hall became race central for the Middle School Science Bowl hydrogen fuel-cell car competition.

Evans Middle School of Ottumwa edged out LeMars 34-26 to win the Middle School Science Bowl. Council Bluffs St. Albert was third and Home Schools of Eastern Iowa was fourth. Ogden put on a strong finish to beat South Hamilton in the hydrogen fuel-cell car race portion of the competition.

Evans' victory means the school will participate in the National Middle School Science Bowl for the second time in three years. Evans won the Ames Lab/ISU Regional in 2006 and went on to finish fourth out of the 25 teams competing in the National Science Bowl event that year. This year's team of Lily Elbaum, Jianwa Bennett, Sarah Beadle, Jacob Huebener and Tivy Wixom will travel to Golden, Colo., June 19-22 for the National Middle School Science Bowl.

Members of the Cedar Rapids-Marion Home Schools team are all smiles as they cruise to victory in the High School Science Bowl.



"Catch me if you can," seems the appropriate quote as the Pella Christian team's car flies across the finish line at the Middle School Science Bowl.

Bioinspiration

Bacteria provide a method for synthesizing magnetic nanoparticles

BY KERRY GIBSON

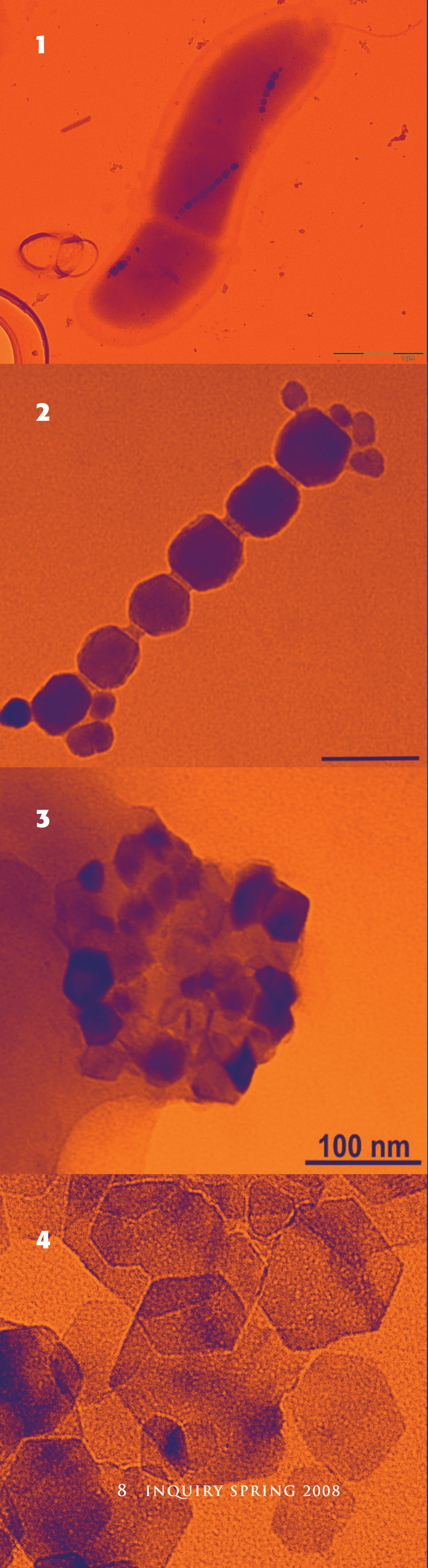
When it comes to designing something, it's hard to find a better source of inspiration than Mother Nature. Using that principle, a diverse, interdisciplinary group of Ames Laboratory researchers is mimicking bacteria to synthesize magnetic nanoparticles that could be used for drug targeting and delivery, as magnetic seals in motors or in magnetic inks and high-density memory devices.

Commercial room-temperature synthesis of ferromagnetic nanoparticles is difficult because the particles form rapidly, resulting in agglomerated clusters of particles with less than ideal crystalline and magnetic properties. Size also matters. As particles get smaller, their magnetic properties, particularly with regard to temperature, also diminish.

However, several strains of bacteria produce magnetite (Fe_3O_4) – fine, uniform nanoparticles that have desirable magnetic properties. These magnetotactic bacteria use a protein to form crystalline particles about 50 nanometers in size. These crystals are bound by membranes to form chains of particles that the bacteria use like a compass needle to orient themselves with the Earth's magnetic field.

To see if researchers could learn from the bacteria, Surya Mallapragada, Ames Laboratory Materials Chemistry and Biomolecular Materials program director, pulled together a team that included microbiologists, biochemists, materials chemists, chemical engineers, materials scientists and physicists from Ames Laboratory and Iowa State University.

As a starting point, former ISU microbiologist Dennis Bazylinski, now at the University of Nevada-Las Vegas, isolated several strains of magnetotactic bacteria for use in the study.



Transmission electron micrographs of **1.** Magnetospirillum magneticum *strain AMB-1 with a chain of magnetosomes inside;* **2.** *nanocrystalline magnetite chain harvested from lysed bacteria (here magnetite nanocrystals are held together by a thin phospholipid membrane material after lysis);* **3.** *protein-templated magnetite nanocrystals of comparable size and morphology;* **4.** *cobalt-ferrite magnetite crystals formed using conjugated Mms6.*

This chain of magnetite particles in M. magneticum *strain AMB-1 after lysis appears to have a sense of humor or at least a friendly disposition.*

Based on earlier work by a Japanese research team, Ames Laboratory biochemist Marit Nilsen-Hamilton looked at several proteins known to bind iron, including Mms6 found in magnetotactic bacteria, which she cloned from the bacteria.

"This protein is associated with the membranes that surround the magnetite crystals," Nilsen-Hamilton says, "and each bacterium appears to make particles with their own unique crystal structure."

Ames Lab chemist Tanya Prozorov tried synthesizing crystals, using the proteins with various concentrations of reagents in an aqueous solution, but the particles formed quickly, were small and lacked specific crystal morphology. At the suggestion of Ames Lab senior physicist and crystal growth expert Paul Canfield, the team used polymer gels developed by Mallapragada and Balaji Narasimhan, who are both Ames Lab scientists as well as ISU chemical engineers, to slow down the reaction and help control formation of the nanocrystals and minimize aggregation.

"It's simple chemistry," Prozorov says, "and you can judge the reaction by the color, watching it go from yellow to green to black as the crystals form. Once the crystals precipitate out, we use a magnet to concentrate the particles at the bottom of the flask, then separate them out to study them further."

Prozorov also conducted electron microscopy analysis of the synthetic nanoparticles, which showed that Mms6 produced well-formed, faceted crystals resembling those produced naturally by the bacteria. Powder X-ray diffraction studies verified the crystal structure of the particles.

Ames Lab physicist Ruslan Prozorov tested the magnetic properties of the synthetic crystals, which also showed striking similarities to the bacteria-produced crystals and bulk magnetite. In addition, the magnetic studies showed that the "chains" of particles formed by the bacteria had a much sharper magnetic transition definition at a higher temperature than single crystals.

"Nature found a way to beat the thermodynamics (of crystalline magnetite) by arranging the nanoparticles in such a way that they aren't affected by temperature the way individual crystals are," Ruslan Prozorov says.

With this basic understanding of magnetotactic bacteria and the ability to synthesize magnetite nanoparticles, the team proceeded to find out if the bioinspired approach could be used to produce cobalt-ferrite nanoparticles. Cobalt-ferrite, which doesn't occur in living organisms, has more desirable magnetic properties than magnetite, yet presents the same problems for commercially producing nano-scale particles.

In addition to their previous method, the team took the added step of covalently attaching the Mms6 to a strand of functionalized polymer known to self-assemble and form thermoreversible gels. Because the polymer strands come together in a particular way, the attached proteins had a specific alignment that the researchers hoped would serve as a template for the formation of cobalt-ferrite crystals. And the way in which the gel formed would help control the speed of the reaction.

"It worked rather well," Tanya Prozorov says, "and we ended up with very nice hexagonal cobalt ferrite crystals." She adds that she is studying whether the protein will also work for the other neodymium, gadolinium, and holmium ferrites.

The research has generated fodder for a number of journal articles, including published works in *ACSNano, Physical Review B* and *Advanced Functional Materials*. The next phase will involve theoretical physicists who will try to develop a model to explain the experimental results.

"This is an exciting interdisciplinary project addressing some of Basic Energy Sciences 'grand challenges' by bringing together materials scientists, chemists, physicists and biologists to develop new bioinspired materials of relevance to DOE's mission," says Mallapragada. "Ames Laboratory is a wonderful environment in which to foster and grow these sorts of interdisciplinary initiatives because teamwork is really built into the culture here."

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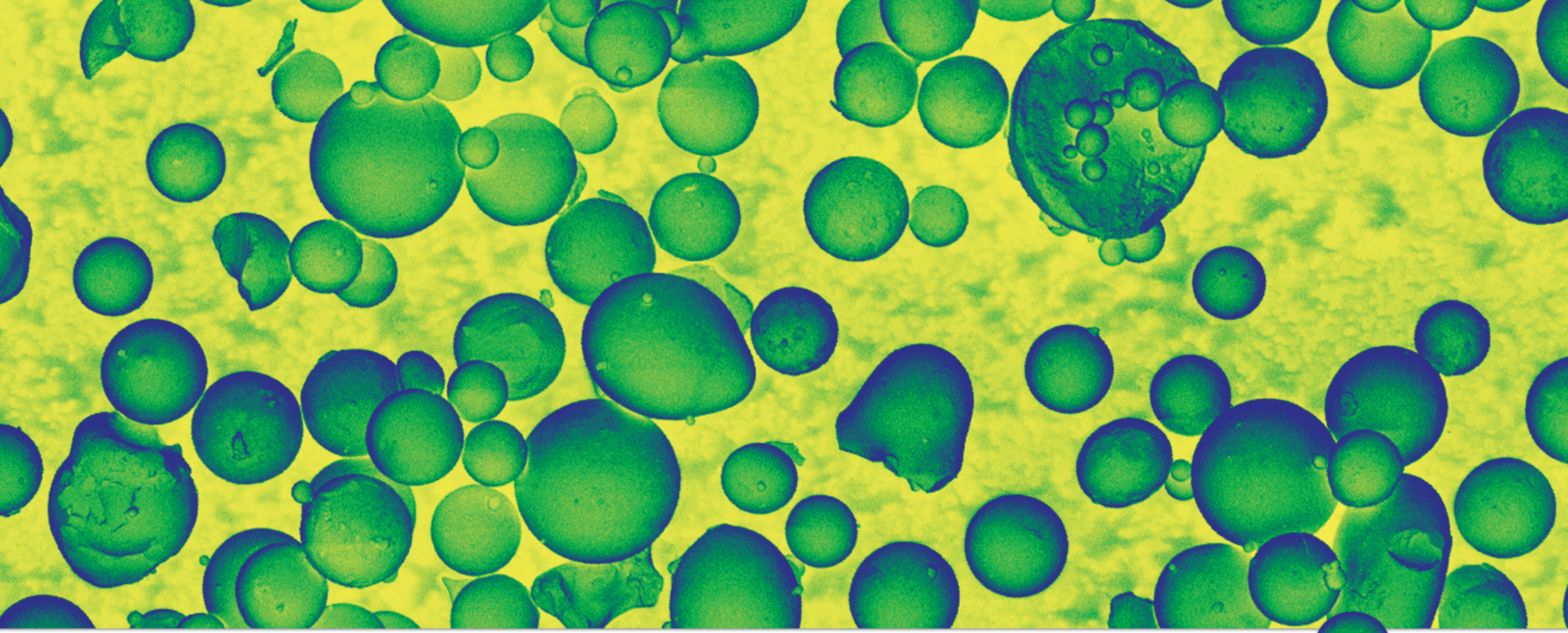

These fine, spherical 2-14-1 permanent magnet alloy powders produced by argon gas atomization may lead to more efficient and economical electric drive motors for ultragreen vehicles.

"Beefing" Up Magnets

For Electric-Drive Cars

BY SAREN JOHNSTON

New magnet alloy stays strong – even at 200 degrees Celsius

ASK IVER ANDERSON ABOUT CONSUMER interest in and desire for "ultragreen" electric-drive vehicles, and he'll reply without a moment's hesitation that the trend is unstoppable and growing fast.

The Ames Lab senior metallurgist and Iowa State University adjunct professor of materials science and engineering is playing a major role in advancing electric drive-motor technology to meet the enormous swell in consumer demand expected over the next five years. He and his Ames Lab colleagues, Bill McCallum and Matthew Kramer, have designed a high-performance permanent magnet alloy that operates with good magnetic strength at 200 degrees Celsius, or 392 degrees Fahrenheit, to help make electric drive motors more efficient and cost-effective. The work is part of the U.S. Department of Energy's Vehicle Technologies Program to develop more energy-efficient and environmentally friendly highway transportation technologies that will enable America to use less petroleum.

Anderson explains that future ultragreen vehicles include fully electric cars, fuel-cell automobiles and plug-in hybrids. "They all have electric drive motors, so that's a common theme," he says. "It's important that those motors be made economically with an operating envelope that fits how they will be driven. The automotive companies in this country have set a series of parameters that they would like electric motors to meet."

One of those constraints being addressed by Anderson and his colleagues is the need for permanent-magnet electric motors to operate well at temperatures up to 200 degrees Celsius. "That raised a lot of eyebrows for people who know anything about magnets," says Anderson. He explains that the most desirable permanent-magnet materials are neodymium-iron-boron magnet materials based on a 2-14-1 crystal structure – $Nd_2Fe_{14}B$. "Most of those types of magnets tend to lose a lot of their magnetic energy at fairly modest temperatures and are operating at much less than half of their power by the time they reach 100 C to 125 C," he says. "So our challenge was to design a high-performance 2-14-1 permanent-magnet alloy that would operate with good magnetic strength at 200 C."

Meeting that challenge, Anderson, McCallum and Kramer designed an alloy that replaces pure neodymium with a mixed rare earth. "We used a combination of neodymium, yttrium and dysprosium because they all form 2-14-1 crystal structures," says Anderson. "Together they have much less degradation of their magnetic properties with temperature due to the influence of the yttrium and dysprosium. Our concept, put forth in our patent application, is that the mixed rare earth 2-14-1 phase would have a lower temperature coefficient." (The relative change of a physical property, e.g., coercivity, when the temperature is changed by 1 Kelvin.)

Once they had tweaked the new alloy to perfection, the researchers next processed it into a fine, spherical powder form using gas atomization, a technique in which kinetic energy from supersonic jets of gas is transferred to a stream of liquid metal, causing it to break up into droplets. "This method best fits the needs of the automobile industry because they want to make their motors by a very high-volume manufacturing process, and that method is injection molding," explains Anderson. Injection molding forms objects from a blended mixture of plastic and metal powder by heating this molding compound to a fluid state and injecting it into a mold.

Stressing the importance of being able to use the injection-molding manufacturing process, Anderson says, "Currently, each magnet making up the magnet array in an electric motor is glued in by hand. That's fine for small runs of 50,000 automobiles, but try doing that for the millions of cars with electric drive motors – one for the front and one for the back – that consumers will want to buy in the next 10 years," he says. "It's not going to work."

Anderson and his colleagues have been refining and pushing the 2-14-1 alloy composition to be more suitable for the rapid solidification that happens in the atomized powder droplets and, ultimately, for the injection-molding process. "We've succeeded in getting very nice properties for these fine spherical powders," he says. He notes that in comparing their powders to spherical commercial powders of larger size, he and his colleagues look at the "crossover temperature" at which the properties of their magnet powders become better than the commercial powders for higher temperature uses. "It used to be 175 C," he says, "but now we've moved that crossover temperature down to the neighborhood of 75 C, which is a tremendous accomplishment. We're very happy about that."

Anderson says they now have what they think is a really good alloy, and also have switched from helium gas to argon gas in the atomization process, which makes the powder-making process a lot cheaper. "That's a move in the right direction for the purposes of commercialization," he says, "and that's what we've been driving for." (No pun intended.)

Reflecting on the goals of the Vehicle Technologies Program, Anderson says, "We need to support our auto companies and help them develop better products. We can do that by getting things worked out at the basic science end – that's our job."

Pictured with the high-pressure gas atomization equipment used to produce the powdered metal are: (from left) Matt Kramer, Kevin Dennis, Iver Anderson, Nathaniel Oster (top), Wei Tang, Yaqiao Wu and Bill McCallum.

Summing up the effort he and his colleagues have made in that regard, he adds, "You can think of this alloy design work as the fundamental end of extending the temperature range of 2-14-1 magnet alloys. Then, we're also working on the process end, which is a fundamental rapid solidification effort to develop the solidified microstructure that will carry the best magnetic properties over in a form that can be mass-produced. You can call this 'use-inspired' research, for sure. And there's an urgent need for this in our society."

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“Good Materials Lead to Good Science”

BY BREEHAN GERLEMAN LUCCHESI

Ames Lab interdisciplinary research group seeks to expand materials synthesis capabilities

AMES LABORATORY EXPERTS IN MATERIALS synthesis and characterization have joined forces in a new research group to advance the Lab’s ability to grow and study high-purity, high-quality crystal samples.

Materials and Engineering Physics Program Director Thomas Lograsso, senior physicist Paul Canfield and senior metallurgist Bill McCallum have formed the Rational Growth, Control and Modification of Novel Materials research group to close the loop between materials characterization and synthesis and, ultimately, expand the range of techniques for growing and studying materials.

Lograsso sat down with *Inquiry* to discuss the new research team.

Inquiry: **What are the overall goals of the new Rational Growth, Control, and Modification of Novel Materials group?**

Lograsso: Ames Lab was founded on high-purity synthesis, and we’ve maintained a high level of expertise and experience. Whether it’s the rare-earth metals or any other material, we pride ourselves on knowing that we are doing the best science on the best materials. And, if we come to find out that materials can be improved, then we improve them to make sure that high-quality materials continue to be our unique niche. I think the continued focus on producing the best materials is the most important and exciting thing that will come out of this new research group.

So we’re bringing together characterization and synthesis so we can more easily make the connection between the best science and the best materials. Good materials lead to good science. But, doing good science on bad samples is just as easy as doing good science on good samples. The difficult part is getting the good samples. That’s where the new Rational Growth research group comes in.

It’s rare to have all the tools and expertise in one spot like we have here at Ames Lab.

Paul Canfield brings his expertise in solution growth of single crystals and in characterization of thermodynamic, magnetic and transport properties of materials. Bill McCallum also has expertise in those types of characterization methods, and he has experience developing processing techniques. I will focus on enhancing several types of synthesis methods and offer my expertise in single-crystal characterization like X-ray diffraction. We each bring a different set of skills to the table to form this interdisciplinary group.

Our effort combines broad research interests that cover a wide range of physical phenomena and ground states, property mechanisms and methods to manipulate that property. Among the three of us, we also have a diversity of material growth techniques, extensive experience in developing new growth techniques and pushing the limits of the ones we already have, and a broad range of characterization techniques that we can use to inform the material design, growth and discovery process.

With that in mind, we have three main goals for our group. The first is to advance the ability to synthesize and characterize high-purity, high-quality materials, mostly in single crystal form, and the second is to quantify and control the synthesis-structure-property relationships, which are the basic science of how chemical inhomogeneities and structural defects affect the properties of responsive materials. Third, we want to explore promising phase spaces that we see as compelling based on advances in synthesis of novel materials.

Overall, we’re focused, as always, on making high-quality crystals. But “high quality” means different things depending on what kind of science you are doing. Sometimes high quality can mean a crystal with minimal defects or a crystal with chemical or phase homogeneity. But, at the heart of the term high quality is the processing-structure-property relationship for any given material. This relationship is always important, but it becomes more important in responsive materials, which are the materials we are going to work with.

In the Rational Growth group, we’ve closed the loop between the synthesizer and the characterizer here at Ames Lab to help best understand and use the synthesis-structure-property relationships.

Why is bringing together synthesis and characterization important?

The people who make materials must understand how synthesis affects structure and properties, and the ability we have here at Ames Lab to connect each part of the synthesis-structure-property relationship is exceptional. It's not just enough to grow a crystal. Characterization of the crystal is of vital importance for two different reasons. The first and obvious reason is to measure its properties, its structure, perhaps the nature of the defects and their population.

Secondly we need then to utilize this detailed characterization information to improve our control over the synthesis process. Such feedback is important, because, again, if you are trying to study some particular behavior, some particular fundamental question of physics or chemistry, defects in synthesized materials are going to affect that measurement. And as one gains a better understanding of the origin of that behavior, then one begins to ask "how do I control the defect(s) that may be affecting that behavior?" So, materials behavior is elucidated through characterization, and, in turn, characterization has to inform the synthesis methods so that you can control and manipulate the materials' behavior.

What kind of new possibilities does the Rational Growth research effort bring about?

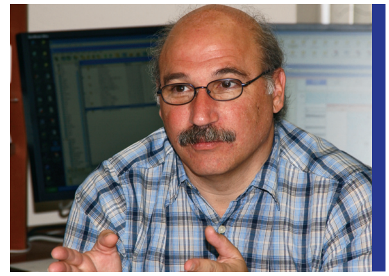
I've been collaborating with a lot of other scientists at the Lab for years, developing crystal-growth protocols and supplying crystals for research. My team could attack specific types of materials, but we were limited somewhat in expanding into other areas or searching for new materials and new types of synthesis due to a limited number of techniques. The particular synthesis method or process often defines the materials on which our group could focus our attention.

But now, in the consolidated research group, we can apply what we learn about growth mechanisms and have the freedom to expand our synthesis methods in a more general way.

The Rational Growth group will expand into new synthesis techniques not typically done in the Materials and Engineering Physics program, such as optical float zoning, vapor transport and solution growth, the latter through a closer working relationship with Paul Canfield.

And forming this team allows us to submit a proposal for advanced crystal growth furnaces that would allow us new flexibility in growth parameters and will, I hope, enhance our capability to work with a broader range of materials.

Likewise, we are pursuing new opportunities by developing those methods required for using reactive materials. Some of the reactive materials can be difficult to work with because they are so air sensitive, and the Rational Growth team wants to have the capabilities which will allow us to do a lot of processing and characterization in an inert environment. Again, that opens up combinations of elements that we, and many others, have not yet been able to consider.



What new synthesis methods do you plan to pursue?

We will advance both the Bridgman and solution growth techniques. In the case of the Bridgman technique, I hope to gain greater dynamic control over nucleation and growth processes that can be optimized to improve uniformity of large single crystals.

We will also be looking to advance solution growth with the aim to understand the limitations of the technique, such as defining growth regimes where proper control of growth can be exercised. The growth regimes are defined in terms of materials and processing parameters, as well as cooling rates and composition. As with the Bridgman technique, the goal is to manipulate the growth processes to achieve single crystals of the desired scientific quality.

We'd also like to expand our repertoire of growth methods to include physical vapor transport. This technique is particularly useful in the synthesis of materials containing volatile constituents, such as arsenic, tellurium, etc. Gaining expertise in handling these components will open up new possibilities in research of superconductors, thermoelectrics and other energy-related materials.

How does the Materials Preparation Center fit in with your effort?

The MPC is a crucial part of our team's research, and we have interacted closely in the past and will continue to do so. The MPC provides the purification processes and other processing to support our research team's goals. The materials and synthesis protocols we discover in the Rational Growth group are then, in turn, transferred into the MPC, where we can make these materials available to the broader DOE community and researchers worldwide.

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BY KERRY GIBSON

Like water through a straw

Parallel cylindrical water nanochannels may explain how fuel-cell membranes work

FUEL-CELL CARS ARE REACHING COMMERCIAL viability in today's increasingly eco-conscious society, but despite their promise, even scientists have struggled to explain just how the fuel-cell's central component – the proton exchange membrane – really works.

However, Ames Laboratory chemists Klaus Schmidt-Rohr and Qiang Chen have offered a new model that provides the best explanation to date for the membrane's structure and how it functions. And armed with that information, scientists should be able to build similar fuel-cell membrane materials that are less expensive or have different properties, such as higher operating temperatures.

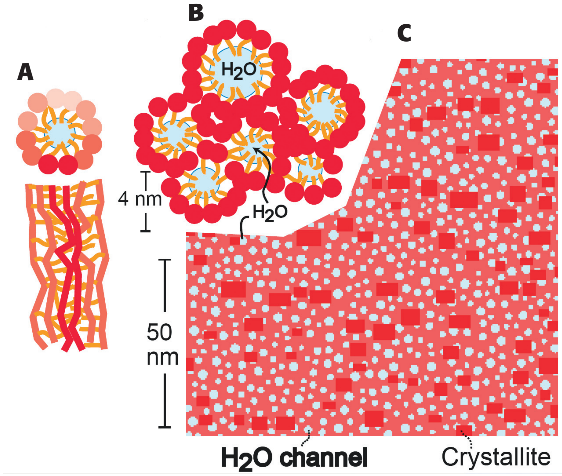
A fuel cell works by pumping hydrogen gas through the proton exchange membrane. In the process, the hydrogen gives up electrons in the form of electricity, then combines with oxygen gas to form water as the byproduct. It can also work in reverse – when current is applied, water is split into its component gases, hydrogen and oxygen.

The model proposed by Schmidt-Rohr and Chen, and detailed in the December 2007 issue of the journal *Nature Materials*, looked specifically at Nafion®, a widely used perfluorinated polymer film that stands out for its high selective permeability to water and protons. Schmidt-Rohr, who is also a professor of chemistry at Iowa State University, suggests that Nafion® has a closely packed network of nanoscale cylindrical water channels running in parallel through the material.

"From nuclear magnetic resonance, or NMR, we know that Nafion® molecules have a rigid backbone structure with hair-like 'defects' along the chain," Schmidt-Rohr says, "but we didn't know just how these molecules were arranged. Some researchers have proposed spheroidal water clusters, others a web-like network of water channels."

"Our theory is that these hydrophobic (water-hating) backbone structures cluster together," he continues, "to form long rigid cylinders about 2.5 nanometers in diameter with the hydrophilic 'hairs' to the inside of the water-filled tubes."

Though the cylinders in different parts of the sample may not align perfectly, they do connect to create water channels passing through the membrane material, which can be 10s of microns thick. It's this structure of relatively wide-diameter channels, densely packed and running mostly parallel through the material that helps explain how water and protons can so easily diffuse through Nafion®, "almost as easily as water passing through water," Schmidt-Rohr says.



A. *Two views of an inverted-micelle cylinder, with the polymer backbones on the outside and the ionic side groups lining the water channel. Shading is used to distinguish chains in front and in the back.* **B.** *Schematic diagram of the approximately hexagonal packing of several inverted-micelle cylinders.* **C.** *Cross-sections through the cylindrical water channels (blue) and the Nafion crystallites (dark red) in the non-crystalline Nafion® matrix (light red).*

To unlock the structure mystery, Schmidt-Rohr turned to mathematical modeling of small-angle X-ray and neutron scattering, or SAXS/SANS. X-ray or neutron radiation is scattered by the sample and the resulting scattering pattern is analyzed to provide information about the size, shape and orientation of the components of the sample on the nanometer scale.

Using an algorithm known as multidimensional Fourier transformation, Schmidt-Rohr was able to show that his model of long, densely packed channels closely matches the known scattering data of Nafion®. Mathematical modeling of other proposed structures, in which the water clusters have other shapes or connectivities, did not match the measured scattering curves.

"Our model also helps explain how conductivity continues even well below the freezing point of water," Schmidt-Rohr says. "While water would freeze in the larger channels, it would continue to diffuse in the smaller-diameter pores."

Schmidt-Rohr adds that additional analysis is needed to determine how the cylinders connect through the membrane.

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BY KERRY GIBSON

Payback Time

Technology transfer efforts paying off big time

IF THE GOAL OF SCIENTIFIC RESEARCH IS to find answers to basic questions, then one of its primary objectives is to take what's learned in the laboratory and pass that knowledge along to business and industry so mankind can benefit from those scientific advances. This transfer of technology is what helps keep the United States competitive in the global marketplace.

One yardstick for measuring success in transferring technology from the lab to the private sector is the amount of revenue generated by the licensing of patented technologies. And against that standard, Ames Laboratory has achieved whopping success over the past few years.

Ames Laboratory has led the Department of Energy's national lab complex – 17 laboratories – in the amount of earned licensing income for the past two years. That's quite an achievement when you compare Ames Lab's annual budget of $30 million with second-place Brookhaven National Laboratory's annual budget of $445 million. In fact, because those revenues exceeded 5 percent of Ames Lab's total annual budget, the Lab has had to turn a portion of that excess back to the U.S. Treasury Department.

"So far as we know, that's the first time that's ever happened," says Deb Covey, Ames Laboratory associate director over Sponsored Research Administration. "We wrote checks for $921,000 in 2006 and $1.03 million this past year."

Covey points out that the earned licensing income is revenue based upon use of the invention, usually a percentage of sales or units sold from products that are actually in the marketplace. This differs from total licensing income that includes earned licensing income, but may also include license issue fees, maintenance fees, milestone payments, paid-up license fees, minimum annual royalties and similar fees.

Since record keeping began in 1980, Ames Lab researchers have been issued a total of 212 patents for 151 different technologies. The most successful to date has been the lead-free solder formula developed by senior metallurgist Iver Anderson's research group. The silver-tin-copper solder is licensed to more than 60 companies worldwide and has generated almost $19 million in royalties. Various iterations of Ed Yeung's R&D 100 award-winning capillary electrophoresis technology have also brought in substantial royalties over the years.

"It doesn't happen overnight," Covey says. "Lead-free solder was originally patented in 1996, and it's only been in the past few years that we've seen the major benefits of that work. We appreciate that we've been lucky and that the timing was right to meet a real need."

At least part of the success of the Lab's licensing efforts lies with the Iowa State University Research Foundation, which protects intellectual property developed on campus, including discoveries at Ames Lab. While other larger DOE national laboratories typically have patent attorneys on staff, ISURF files patent applications, licenses intellectual property and monitors for patent infringement for Ames Lab.

If and when license royalties flow back to ISU, ISURF recoups the cost of patenting the invention and takes an administrative fee off the top to cover other expenses. One third of the remaining money goes to the inventors, while Ames Lab and ISU receive 51 and 49 percent of the balance respectively; up to the 5 percent of the Lab's budget.

"We're restricted on how we can spend that money," Covey says. "It has to be used for science, education or tech transfer, and it's primarily for new science." She adds that seed funding for collaborative research is one way the Lab has made a concerted effort to encourage development of new ideas that may need a proof of concept in order to pursue DOE or other funding.

"It's great that we're able to capitalize on our successes by funding new research efforts," Covey says. "It also demonstrates the importance of protecting the discoveries our researchers make because you never know what might be the next big success."

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