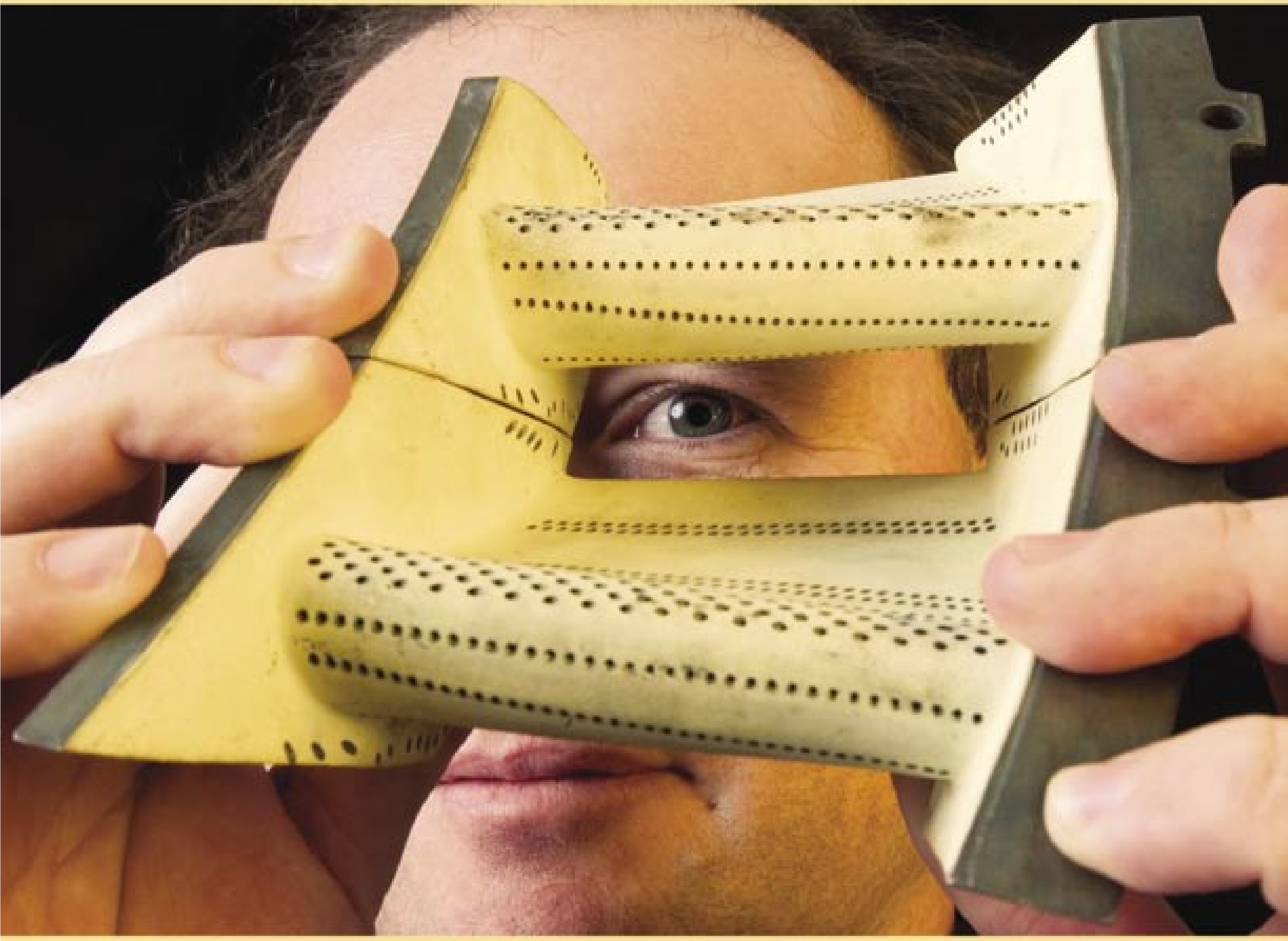
Inquiry 2005

Science and Technology at the Ames Laboratory

Award-winning bond coat

A photonic first

Inside a fuel-cell membrane



AMES LABORATORY

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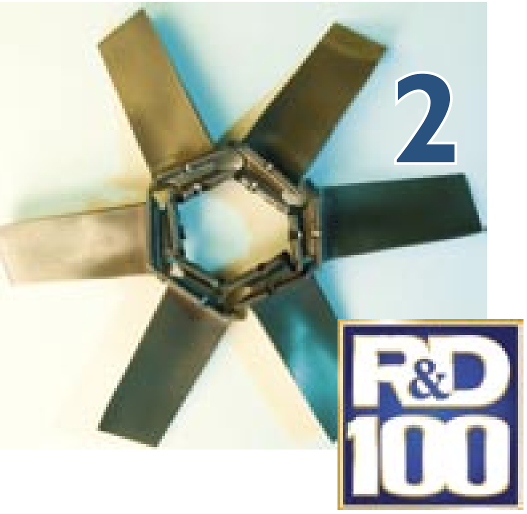
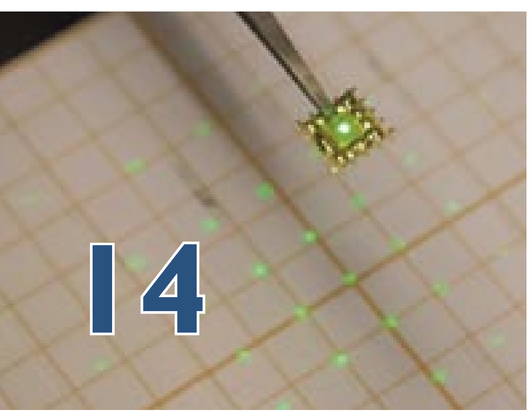
Contents





(front cover) With an eye to the future, Brian Gleeson, along with co-principal investigator Dan Sordelet, is developing a new bond coat for thermal barrier coatings that will allow engine components, such as the turbine blade he is holding, operate more successfully in severe, high-temperature environments.

(back cover) A "treasure hunt" for interesting photos led to the discovery of these shiny circles found scattered and abandoned in a laboratory drawer. The eye-catching hoops are actually the concentric rings and cover for a steam bath.

from the Director

We are pleased to begin this issue of *Inquiry* with both a thank-you and a note of congratulations. Our thanks go to Secretary of Energy Samuel Bodman for his visit to the Ames Laboratory in June, only four months after assuming the duties of Secretary. The Secretary was extremely impressed with the several scientific presentations by Ames Laboratory researchers. He also expressed his high regard for the national labs in maintaining the nation's leadership in science and technology.

Secretary Bodman (left) and Tom Barton

Our congratulations go to Brian Gleeson, director of Ames Lab's Materials and Engineering Physics Program, and Dan Sordelet, senior scientist, for winning a 2005 R&D 100 Award. Brian and Dan have developed novel platinum-modified nickel-aluminide bond coats for thermal barrier coatings. The new bond coats promise to greatly improve the durability of gas turbine engines, allowing them to operate at higher temperatures. Their award-winning work leads the stories in this year's *Inquiry*.

Ames Laboratory scientists continued to carry out innovative basic and applied research in a variety of scientific areas during the past year. Outstanding work led by Kai-Ming Ho and Kristen Constant brought together the disciplines of condensed matter physics and materials engineering to significantly advance research on photonic bandgap crystals. Their unique modification of a technique known as "microtransfer molding" may considerably reduce the costs of fabricating photonic crystals.

An example of basic research is being carried out by Bill McCallum and a team of researchers from across the Lab. The group is studying a series of praseodymium-nickel-silicon compounds to determine the relationship between molecular structure and important magnetic properties, such as magnetorestriction. The hope is that these compounds can serve as a theoretical model for understanding other rare earth-nickel-silicon alloys and for enhancing their potential uses.

In the Laboratory's Scalable Computing Lab, Masha Sosonkina is developing adaptive algorithms to execute high-performance applications efficiently in dynamically changing computing environments. In particular, she has been working on a co-scheduler for GAMESS, a computational chemistry code, to make the simultaneous execution of GAMESS calculations more efficient.

Getting into the "fuel of the future" game, Vitalij Pecharsky and a team of Ames Lab researchers will be investigating complex hydrides in an effort to help solve the problem of hydrogen fuel storage – how to carry enough hydrogen onboard a vehicle to travel even moderate distances between refueling stops. The work is the focus of $1.6 million in funding awarded to Ames Laboratory from the DOE's $64 million Hydrogen Fuel Initiative.

As you read about these intriguing research efforts in the 2005 *Inquiry*, I'm sure you'll agree that Ames Laboratory scientists are engaged in some very exciting activities in their efforts to find solutions to our nation's energy problems.

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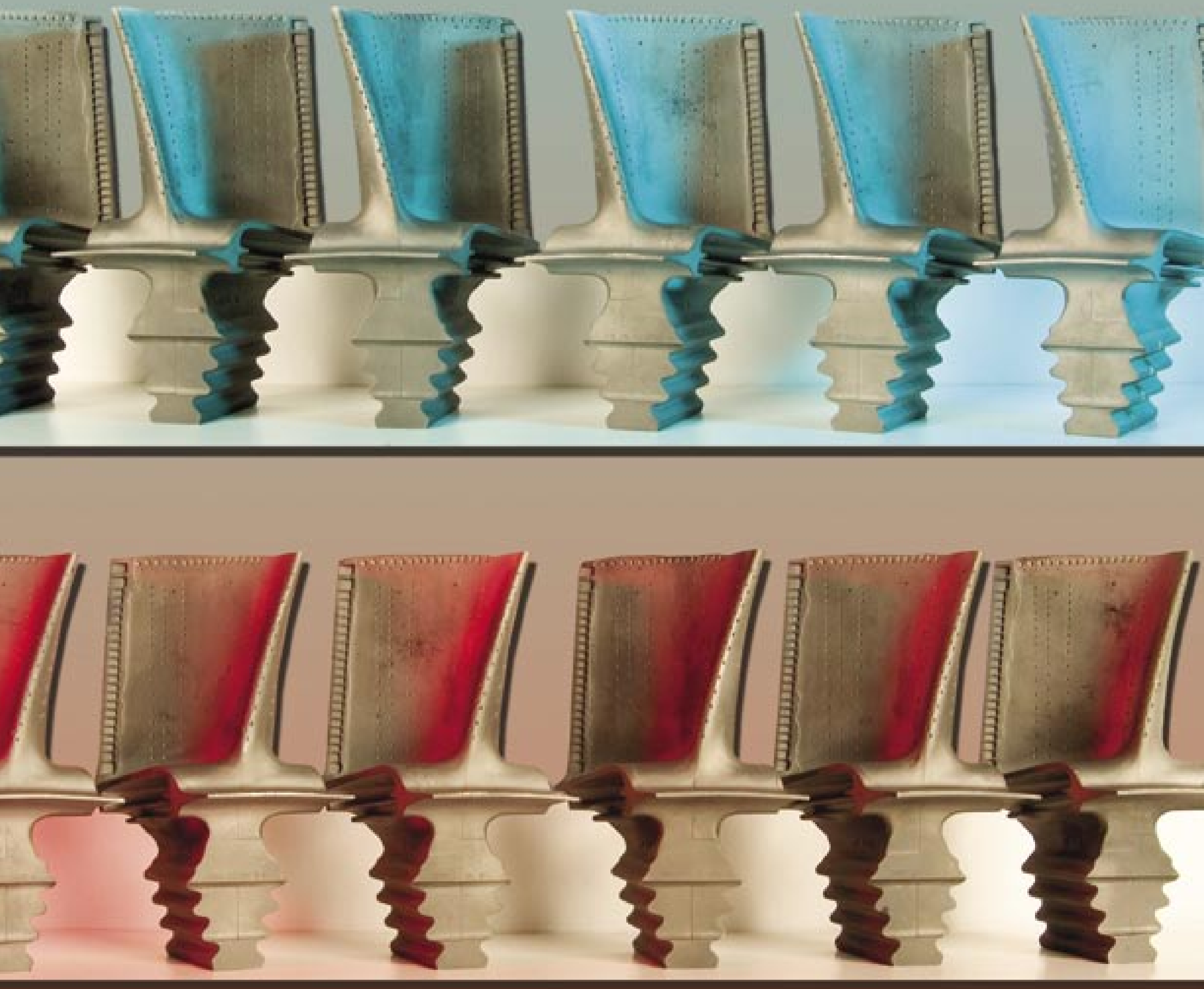
Beating the Heat

A new bond coat may mean longer life for gas turbine engines

by Saren Johnston



Dan Sordelet and Brian Gleeson's new bond coat for thermal barrier coating systems will allow higher operating efficiencies for gas turbine blades in aircraft engines.

A unique bond coat composition developed by Dan Sordelet (left) and Brian Gleeson may one day become the standard in thermal barrier coatings that protect gas turbine blades, like the ones they're holding, from heat damage.

Flying from coast to coast or country to country has become a matter of routine for many people in today's fast-paced, workaday world. And frequent flyers have learned to take advantage of their valuable in-air time while jetting through the skies at 300-400 miles per hour. Some strategize delicate business maneuvers or scrutinize stock portfolios, while others mentally rehearse invited talks or happily succumb to the intrigue of a Dan Brown novel. All this and more airline passengers can accomplish at 30,000 feet, compliments of the hardworking gas turbine engines that keep their carriers of choice up there in the "friendly skies."

Not surprisingly, then, along with all the dependency on air travel that today's "commuter" has developed, there has come a steady demand for better, more efficient gas turbine engines that can operate at elevated temperatures. Addressing that need, Ames Laboratory and Iowa State University researchers have developed a new bond coat for thermal barrier coatings, or TBCs, that may allow gas turbine engines in aircraft and other power-generating technologies to better withstand severe, high-temperature environments. The basic research effort could provide a TBC system with significantly improved reliability and durability of turbine blades, thus enabling higher operating efficiencies and extending engine lifetimes.

Just what is a TBC?

Commercial thermal barrier coatings consist of three layers. The first layer is typically an aluminum-rich bond coat that is based on the compound nickel-aluminum, or NiAl. The bond coat is applied directly to the turbine blade. The second layer is a thin, thermally grown oxide, or TGO, which forms as the aluminum in the bond coat oxidizes. The third layer, a thin (around half a millimeter) ceramic top coat, has a low thermal conductivity and, therefore, acts as a barrier against heat damage.

"By applying a thermal barrier coating to a turbine blade, it is possible to increase the combustion temperature of the engine, which leads to significantly improved efficiency in gas turbines," says Dan Sordelet, an Ames Laboratory senior scientist. He explains that the ability of the bond coat to oxidize and form a continuous, slow-growing and adherent TGO layer is critical to creating a resilient and reliable thermal barrier coating.

Things can and do go wrong

Sordelet emphasizes that cracking or breaking apart of the TGO layer due to time and service in a severe environment is one of the main causes of failure in a TBC system and the associated engine components. Also, at temperatures around 1100 degrees Celsius (2012 degrees Fahrenheit) and above, the aluminum in the bond coat begins to diffuse more rapidly into the substrate, changing the overall bond coat composition.

"If enough aluminum diffuses into the substrate, eventually a phase change, which is a change in the crystal structure, occurs and can lead to large-scale distortion of the bond coat surface and subsequent failure of the TBC system," says Sordelet. Elaborating, he adds, "Initially, there is a very thin TGO layer sitting on a very flat bond coat surface. If the bond coat continues to lose aluminum so that phase transformations take place, conditions will change from thin and flat to thin and 'rumpled.' Stresses develop, and the likelihood for the top coat to come off increases rapidly."

Understanding the alloy – the platinum bonus

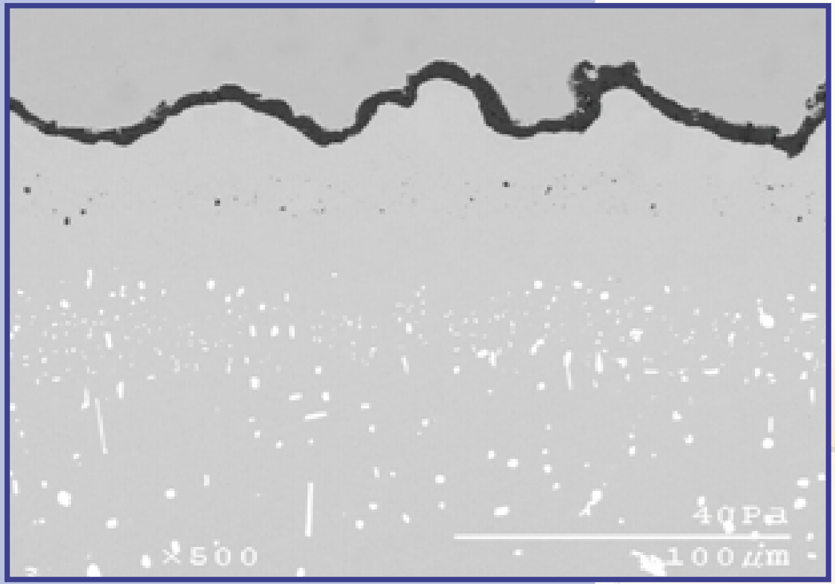
Working to improve the reliability of TBC systems, Sordelet and Brian Gleeson, director of Ames Laboratory's Materials and Engineering Physics Program and an ISU professor of materials science and engineering, have performed experiments on various nickel-aluminum-platinum, or Ni-Al-Pt, alloy samples made by Ames Laboratory's world-renowned Materials Preparation Center.

"Dan and I received funding from the Office of Naval Research to conduct fundamental research on the Ni-Al-Pt system, including experimental determination of isothermal phase diagrams," says Gleeson. "The phase diagrams provided much-needed guidance for elucidating the relationships between phase constitution/composition and properties in this system."

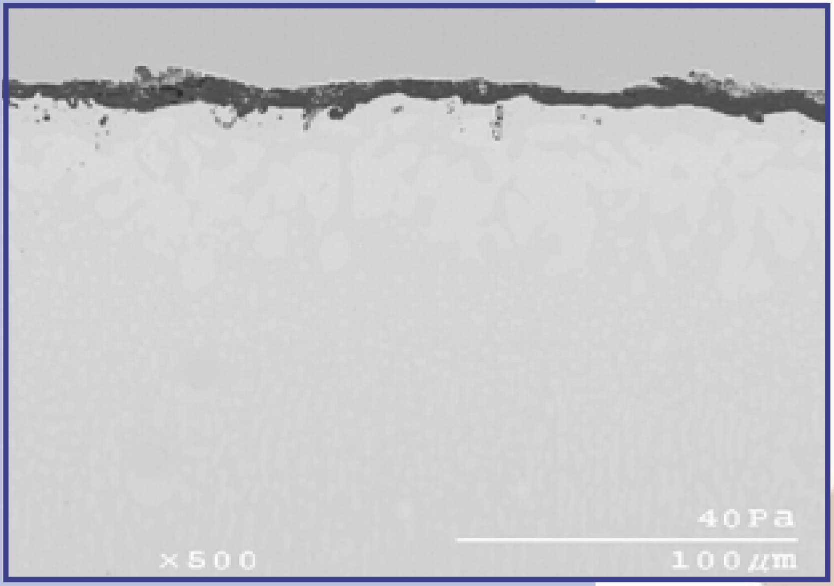
Quite unexpectedly, the two researchers found that platinum additions significantly improved the oxidation resistance of nickel-rich bulk alloys having the same type of structure as the turbine alloy. Without platinum, these alloys form a relatively fast-growing TGO scale that is prone to spall, or break up, during thermal cycling. By adding platinum, the alloys become highly resistant to oxidation, forming a tenacious, slow-growing TGO scale. But Sordelet and Gleeson weren't satisfied yet.

A little dab will do

"In the typical design of alloys for oxidation resistance, you always find that adding a little sprinkle of this and a little sprinkle of that can have dramatic effects," says Sordelet. "Well, Brian's intuition to sprinkle either zirconium or hafnium was remarkably accurate." As the researchers



This electron microscope image of a commercial bond coat after thermal cycling shows how the thermally grown oxide becomes "rumpled," leading to subsequent spallation of the ceramic top coat and failure of the entire TBC system.



This electron microscope image of the new Ames Lab/ISU bond coat composition after an identical number of thermal cycles shows essentially the same surface topography as the starting surface (i.e., no rumpling).

added a little bit of either or both to the nickel-rich compositions, things improved tremendously.

"With the addition of hafnium, oxidation rates went down by up to an order of magnitude," Sordelet says. "We now have growth rates that are the lowest ever reported. It's quite remarkable!"

In current aluminum-rich bond coat alloys, only a very small amount (e.g., <0.1 wt.%) of zirconium or hafnium may be added to improve oxidation before adding too much is detrimental, causing catastrophic oxidation failure. In commercial coating production, it is extremely difficult to achieve an adequately uniform distribution of such a small amount of metals like these in a cost-effective way.

"Fortunately, in the new nickel-rich bond coat, we have observed significant reductions in oxidation rates over a wide concentration, from 0.5 to 4 wt.% hafnium," Gleeson emphasizes. "These are no longer 'trace' levels to a processing engineer and can thus be easily alloyed homogeneously throughout the material." This attribute gives Sordelet and Gleeson's new coating a huge processing window, which they both say has been very desirable to people they've visited within the coatings industry.

Bulk luck

Their work with the bulk alloys led Gleeson and Sordelet to yet another fortunate result. They discovered that platinum changed the diffusion behavior of aluminum in their nickel-rich compositions.

"Instead of aluminum going from the bond coat down into the substrate, it was moving up from the substrate into the bond coat," explains Gleeson. "This phenomenon is referred to as 'uphill diffusion,' and it's a consequence of the strong chemical interaction between aluminum and platinum. With our new bond coating compositions, the substrate can act as a large reservoir for aluminum and hence maintain the protective growth of the oxide layer."

The two researchers have recently demonstrated that their new coatings can offer significant benefits over current state-of-the-art bond coatings used in advanced TBC systems. "We have been working with an aeroengine manufacturer, and the results to date have been extremely encouraging," says Sordelet.

Brian Gleeson and Dan Sordelet have won a 2005 R&D 100 Award for the development of novel platinum-modified nickel-aluminide coatings that deliver unprecedented oxidation resistance and phase stability as bond coat layers in thermal barrier coatings. The new bond coats promise to significantly improve the reliability and durability of gas turbine engines, allowing them to operate at higher temperatures and extending their lifetimes. The *R&D Magazine* program, now in its 42nd year, honors the top 100 products of technological significance marketed or licensed during the previous calendar year. The winning of an R&D 100 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. Since 1984, Ames Laboratory has earned 15 prestigious R&D 100 Awards.

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Research funded by:

Office of Naval Research

Courting Complex Hydrides

Lab gets $1.6 million to study complex hydrides

by Kerry Gibson

Marek Pruski, left, and Vitalij Pecharsky stand in front of a new nuclear magnetic resonance magnet that Pruski will use to study complex hydride materials. Joining Pruski and Pecharsky on the $1.6 million Hydrogen Fuel Initiative project will be Victor Lin and Scott Chumbly.

Hydrogen is being touted as the fuel of the future, a clean-burning, renewable and inexpensive replacement for petroleum. But a major stumbling block for hydrogen-powered vehicles is figuring out a way to carry enough hydrogen onboard to travel even moderate distances between refueling stops.

A group of Ames Laboratory researchers will be investigating a possible solution to that problem thanks to $1.6 million in funding announced recently by Department of Energy Secretary Samuel Bodman as part of a $64 Million Hydrogen Fuel Initiative. Funding for the project will be spread over three years.

"With compressed hydrogen gas, you simply can't carry a tank big enough to travel very far," Ames Lab senior scientist Vitalij Pecharsky says. "The answer is a hydrogen-rich, solid fuel that mimicks the hydrogen content of methane, where four hydrogen atoms encapsulate a single carbon atom."

Unlocking the hydrogen

So why not just use methane? According to Pecharsky, methane and similar hydrocarbon compounds have covalent bonds that keep the hydrogen atoms tightly "locked" in place. The energy required to break those bonds is very high compared to the energy you'd get from the hydrogen produced. Also, methane and other hydrocarbons that come from oil are not renewable. The ideal solution would be a hydrogen-rich solid material that gives up its hydrogen atoms easily, through moderate heating or by other means. These materials could also be "recharged" – absorbing "new" hydrogen atoms during refueling from a pressurized hydrogen gas source.

That's why Pecharsky and fellow Ames Lab scientists Marek Pruski, Victor Lin and Scott Chumbley are looking at some novel materials – light-metal alanates, borohydrides, amides, imides, and their derivatives – that have a total hydrogen content exceeding 10 percent by weight.

Shaking things up

A key component in the research project is solvent-free mechanochemical processing, a technique Ames Laboratory researchers had shown back in 2002 to work well when applied to complex hydrides. The process uses variable energy milling to modify both the structure and properties of hydrides, and potentially, to make them easily rechargeable with hydrogen. Materials to be processed are placed in a hardened steel vial along with steel balls. The vial is vigorously shaken and mechanical energy transferred into the system alters the crystallinity of the solids and provides mass transfer, eventually breaking down the solids and releasing hydrogen, or combining the materials and hydrogen gas into new compounds.

"Processing these materials without the use of solvents is important," Pecharsky says, "because once a material is dissolved, its structure fundamentally changes. Creating these complex hydride compounds in solid state will allow us to look at the molecular structure to see if there are ways to more easily get the hydrogen back out of these systems."

A mechanical ball mill, similar to the one shown above, is used to create organic compounds without the use of solvents. The materials to be combined are placed in the canister along with the steel balls. Operating similar to a paint shaker, mill shakes the canister and the mechanical energy going into the system is transferred to the materials, eventually combining them at the molecular level.

Keeping it "small"

Another ingredient the group will use is called nanostructuring. Ames Lab chemist Victor Lin has developed a way of using the nanoscale pores in a self-assembling polymer as "molds" to precisely control the size of the material particles going into the milling process. Smaller particles have higher surface energies, and surface energy may be a decisive factor in shifting thermodynamic equilibrium. Lowering the size of particles to a few nanometers also reduces the distances over which the mass transport takes place, thus improving the kinetics – the rates of the reactions – of complex hydride-hydrogen systems.

Synthesizing various combinations and sizes of materials will provide samples to be studied and characterized using a variety of high-tech methods. Ames Lab metallurgist Scott Chumbley hopes that scanning and transmission electron microscopy will give researchers a close-up look at the structure of the processed materials. The team will also rely on the expertise of Ames Lab senior scientist Marek Pruski in using solid-state nuclear magnetic resonance. Earlier studies performed by Pruski's group proved that NMR is uniquely suited for the studies of complex phases resulting from the milling process. Coupled with X-ray powder diffraction and other traditional materials characterization techniques, researchers hope to gain a fundamental understanding of the relationships between the chemical composition, bonding, structure, microstructure, properties and performance of these materials.

"We'll look at the rates of absorption and desorption of hydrogen as well as the cycling properties of these materials at various temperatures and pressures," Pecharsky says. "Furthermore, we plan to modify these nanoparticles with titanium and other transition metal catalysts and perform a full array of characterization and hydrogenation-dehydrogenation property tests on these metal-doped nanostructured hydrides."

Predicting outcomes

Parallel with the materials' characterization, the group will work with physicist Purusottam Jena of Virginia Commonwealth University to develop first-principle theoretical models based on the experimental data. Those models will then be used to predict outcomes of further experiments. The predictions and actual results will be compared to see if the theory holds or needs further modification. Ultimately, the theoretical model will be used to help steer research toward the most promising compounds.

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Research funded by:

Hydrogen Fuel Initiative

What Makes a Fuel-Cell Membrane Tick?

Using NMR to probe Nafion®'s structure

by Kerry Gibson

Qiang Chen prepares to load a sample holder contain a piece of Nafion® membrane into the NMR probe. NMR allows researchers a detailed view of a material's structure in its solid state when the material is non-crystalline in nature and dissolving it would alter the structure.

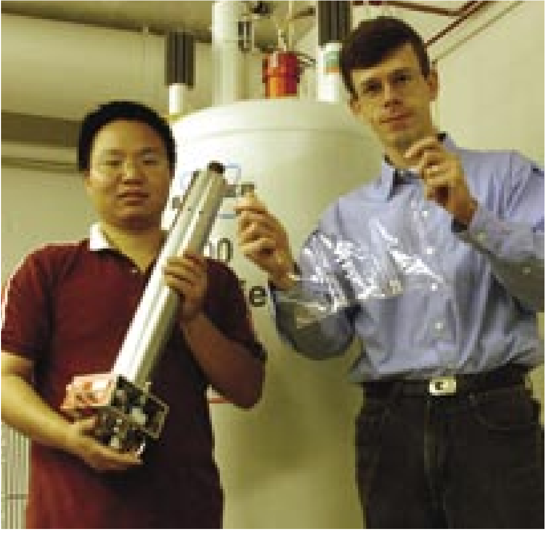
One of the keys to hydrogen fuel-cell technology is a thin, plastic film that "magically" separates water into its component parts of hydrogen and oxygen and at the same time releases electrons that generate power from the fuel cell. The membrane, known commercially as Nafion® (see photo, page 9), looks like a clear, heavy vinyl, but because of what it's able to do, the material is more than worth it's weight in gold.

Developed by DuPont, Nafion® has been around for roughly 30 years and is the commercial standard for the proton exchange membrane in fuel cells. Despite that history and commercial success, surprisingly little is known about its molecular structure or just how it works.

"It takes 24 of these to make a hydrogen fuel cell used in buses," says Ames Laboratory chemist Klaus Schmidt-Rohr, as he held a roughly one-foot-square sheet of Nafion®, "so it costs several thousand dollars just for the membrane material. In order to develop more affordable alternatives, we need to understand the molecular structure of Nafion® and how it works."

NMR probes stucture

Schmidt-Rohr has been studying the membrane material for about five years, primarily using a technique called nuclear magnetic resonance, or NMR. The spectroscopic technique basically involves placing the material within a magnetic field and measuring how energy levels of the atomic nuclei split as the material transitions from one energy state to another. In general, the more complex the structure of the



Klaus Schmidt-Rohr, right, and graduate student Qiang Chen stand in front of the nuclear magnetic resonance chamber. Tiny samples of Nafion® membrane are placed in a probe, which Chen is holding, and lowered into the high magnetic field within the chamber.

material, the sharper or more distinctive its NMR signature will be.

"A material like polystyrene has a broad NMR signature because its structure is amorphous," Schmidt-Rohr says. "Perfluoronated polymers such as Teflon® or Nafion® register these sharp peaks, indicating a surprising amount of order – in other words, a crystalline structure."

According to Schmidt-Rohr, electron scattering techniques can provide an overall view of the structure, while NMR allows "us to go segment-by-segment and look at the structure from the bottom up."

Bent backbones

Previous studies of Teflon® show it has rod-like, helical structures that spin rapidly, about a million times a second. This "backbone" is hydrophobic – water hating – which helps explain its nonstick nature, and the rods pack neatly into parallel bundles.

In his study of Nafion®, Schmidt-Rohr saw a similar backbone pattern with some important differences. The signature line of the backbone showed up nicely, but it had "defects" along the chain approximately every 14 units.

"We thought now that we have these straight (backbone) elements, they'll want to crystallize and pack nicely together," he says. "We did one more experiment and looked at how one local piece is parallel to another. What we found really threw us off because they weren't parallel. They weren't random, but they weren't nicely packed either."

The literature on the structure Nafion® proposed about a dozen different models, but none of them were consistent with the observations of Schmidt-Rohr's NMR studies.

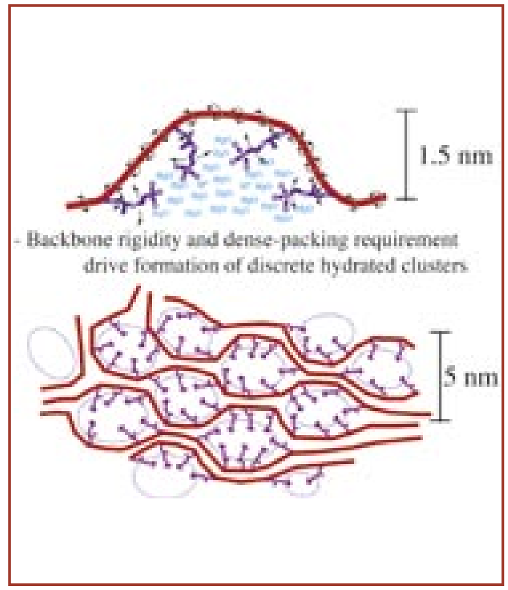
"We discovered these ionic sulfunate side groups with hair-like ends," he says. "These structures are charged and are hydrophilic – they like water – while the backbone is hydrophobic."

New model

Schmidt-Rohr developed what he calls an "alternating curvature model" that shows the backbones aligning along the bends and the hairlike structures clustering together. The material is crystalline in areas where the backbones align, roughly 10 percent of the overall structure. And in order for a polymer chain to have the required stiffness, the theory is that the density of the hairs matches the density of the backbone.

Moreover, the clusters of hydrophilic hairs form pores 3-5 nanometers in size that hold water. The next step is to figure out how the water moves from one pore to the next.

"Nafion® has an extremely high permeability for water," Schmidt-Rohr says, "almost like water moving through water. One important feature that is missing is a channel or means for the water to move between the pores. To figure that out, we'll have to do low-temperature studies to slow the transfer of water."



Based on his findings, Schmidt-Rohr has developed an "alternating curvature" model of Nafion® in which the backbone aligns between bends, and the hairlike structures cluster together to form 3-5 nanometer pores. The hairlike structures are hydrophilic, so water tends to collect in the pores.

Unlocking the structural secrets of Nafion® may help not only in development of materials for fuel-cell membranes but other purposes as well.

"The material has these 3-5 nanometer pores," Schmidt-Rohr says, "so if we were able to fill those with other counter-ions, it could provide optical properties for a variety of nanoscale applications."

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Research funded by:

DOE Office of Basic Energy Sciences
Materials Chemistry Division

Secretary Bodman Visits Ames Lab

Flanked by security personnel and Ames Lab officials, Secretary Bodman (right) begins his Ames Laboratory tour accompanied by Director Tom Barton (center) and Alan Goldman, division director of Science and Technology.

"It is very difficult for me to imagine anyone anywhere who is better qualified to serve our nation as Secretary of Energy than Samuel Bodman," said Ames Laboratory Director Tom Barton as he introduced the Secretary at the all-hands meeting, Friday, June 3. "Leading our nation to a secure energy future is about as daunting a task as I can imagine, frankly, but we are, indeed, fortunate that someone with such incredibly impressive and appropriate credentials as has Secretary Bodman is on the job."

Coming to the podium, the Secretary thanked members of the audience for turning out in such great numbers. "I want you to know that I'm particularly pleased to be here," he said, noting that he was born and raised in the neighboring state of Illinois.

Secretary Bodman explained that he's an engineer and brings that perspective to his job with the Department of Energy. "The national laboratories, like this one, have a special meaning to me," he said. "The laboratories have been enormously productive organizations in helping to maintain our nation's leadership in science and technology. This lab is one of the smaller labs in the group, but that does not reflect on the preeminence of the work that is done here. The work of materials technology I was prepared to believe before I got here is quite extraordinary, and that was reinforced once I arrived."

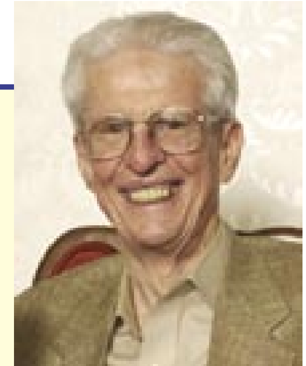
The Secretary expressed his admiration for how well the Lab works on an interdisciplinary basis. "You seem to have perfected that art," he said, praising the Lab's unique ability to integrate students, both graduate and undergraduate, into its research endeavors. Commenting on the fact that student employees account for some 20 percent of the Lab's workforce and that thousands of them have received their degrees while working here, the Secretary said, "That's really extraordinary. It's quite amazing and something to be treasured – something for you to focus on."

Secretary Bodman encouraged the Lab to continue its interest in working on technologies and products that could have commercial possibilities. He emphasized that the partnerships that include government funding in support of science research, the potential commercial partners in these endeavors, research universities, and venture capitalists have, in his opinion, helped create what we call today the American economy. "Without that process, we wouldn't have the economy we have today," he said. "It has been something that the Ames Laboratory seems to have a real focus on in its own way, and I would continue to encourage you to realize and treasure what you have here because it really is something quite special."

Concluding his remarks, Secretary Bodman said, "I'm very pleased and honored to have this job. This is the first time that a person has taken on the job as Secretary of Energy who is burdened by some knowledge of energy," he added, drawing appreciative laughter from the audience. "Hopefully you'll look at me as someone who has some understanding of what to do and how to do it. I've got this job, and I'll be very serious about it," he promised, adding, "I'll count on your help as we go forward."

Senior metallurgist Karl Gschneidner visits with Secretary Bodman about magnetic refrigeration during the Secretary's tour of Ames Laboratory.

Corbett Wins Spedding Award



John Corbett, Ames Laboratory senior chemist, was named the recipient of the 2005 Spedding Award, the top honor for researchers in the field of rare-earth science and named for the first director of Ames Laboratory.

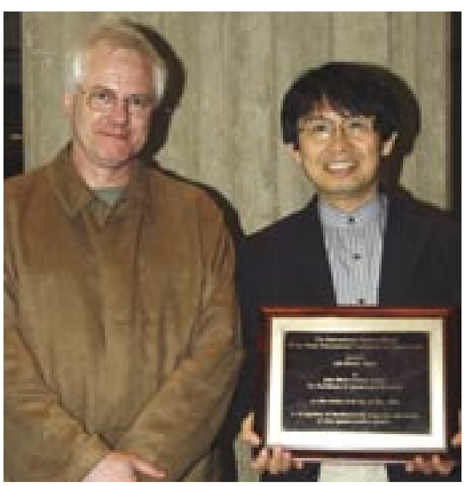
Corbett, who is also a distinguished professor of chemistry in the College of Liberal Arts and Sciences at Iowa State University, is the 11th recipient of the Spedding Award, which is given annually by the Rare Earth Research Conference. The award is given in recognition of excellence and achievement in research centered on the science and technology of rare earths and consists of a medal mounted on a plaque and a prize of $1,000, sponsored by Bracco Research USA Inc.

The award was presented to Corbett at the 24th Rare Earth Research Conference in June in Keystone, Colo. During the conference, Corbett presented an awards lecture on his many years of work with reduced rare-earth metal compounds. Corbett is the third Ames Laboratory researcher to receive the Spedding Award. Senior physicist Sam Legvold was a co-winner of the third award, and senior metallurgist Karl A. Gschneidner was the sixth winner.

The Spedding Award is named in honor of Frank Spedding, a longtime Iowa State chemistry professor and one of the nation's leading atomic scientists. Spedding was a pioneer researcher with rare earths and organized and directed the chemistry phase at Iowa State of the historic Manhattan Project. He founded the Institute for Atomic Research and the Ames Laboratory of what was then the U.S. Atomic Energy Commission.

A member of the National Academy of Sciences, Corbett has been an Ames Laboratory researcher and a faculty member in ISU's chemistry department since 1952. During that time, he has served as a division chief and program director at the Ames Laboratory and as chair of the ISU chemistry department.

Quasicrystal World Focuses on Ames



Jean Marie Dubois, left, stands with An-Pang Tsai who received the first-ever Dubois Award for excellence in quasicrystal research.

More than 200 of the world's leading researchers in the field of quasicrystals gathered in Ames, May 22-26, for the Ninth International Conference on Quasicrystals. Selection of Ames as the host city among the likes of Beijing, Avignon, Tokyo, Stuttgart, Bangalore, and Zurich is testimony to the strength of materials research being conducted at Ames Laboratory and Iowa State University. This year was also only the second time the U.S. has hosted the event since the first conference was held in 1986.

Quasicrystals, the focal point of the conference, are typically aluminum-rich metallic alloys that are somehow able to form into crystals – usually with a five-fold symmetry – in which the atoms are ordered, but without the periodicity common in crystalline materials. Quasicrystalline materials are hard, slippery, poor conductors of heat, and resistant to attack by other chemicals. This makes them particularly useful for applications requiring resistance to wear, low adhesion or a thermal barrier, such as machinery operating in abrasive environments, coatings inside pipelines or cookware, or electrical insulators.

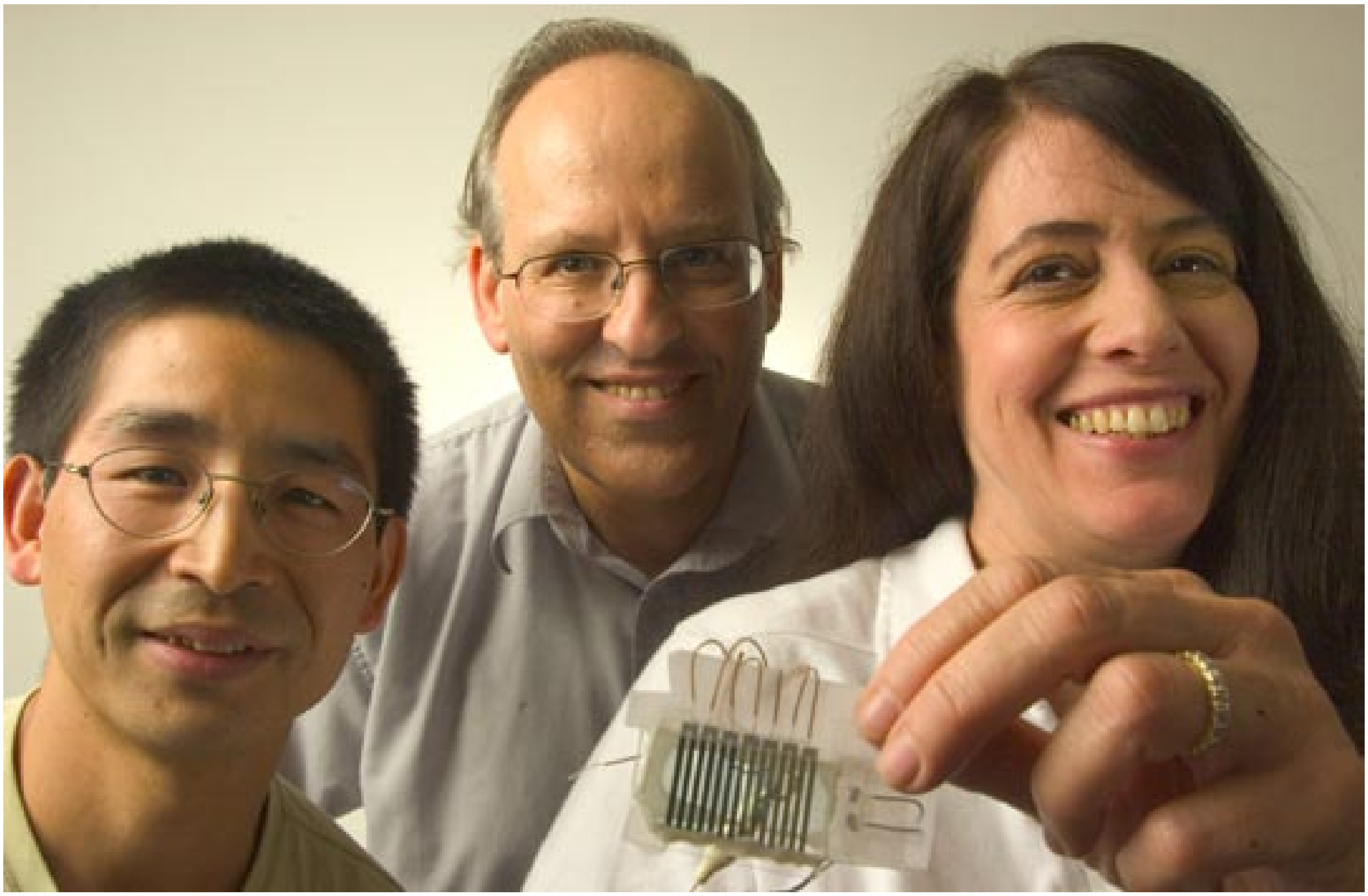
A highlight of the conference was the awarding of the inaugural Jean-Marie Dubois Award, named for one of the key researchers in the field. Dubois, Director of Research at the Centre National de la Recherche Scientifique in Paris, presented during the conference and was recently named as the 2007 winner of The Minerals, Metals & Materials Society's (TMS's) prestigious Robert Franklin Mehl Award.

The Dubois Award was presented to Professor An-Pang Tsai of Sendai University for his "fundamentally important discoveries of new quasicrystalline phases." The award consists of a $2,000 cash prize and a plaque.

Oxygen Monitoring Made Simple

Sound collaboration results in a new sensor company

by Saren Johnston



Joseph Shinar (center), Ruth Shinar and Zhaoqun Zhou are developing a new integrated sensor technology that is expected to result in low-cost sensor (micro)arrays for multianalyte detection.

In the world of sensor technology, oxygen sensors represent a very large, multifaceted and ever-expanding market. The medical industry, alone, accounts for a whopping portion of that market, considering oxygen monitoring is essential to the daily health care regimens of millions of individuals throughout the world. Other fields where oxygen sensors have applications include environmental, biological, food packaging, health and safety, and aerospace.

Now, basic research on the photophysics of luminescent organic thin films and organic light-emitting devices, or OLEDs, by Ames Laboratory senior physicist Joseph Shinar, together with sensor research by Ruth Shinar, a chemist at Iowa State University's Microelectronics Research Center, has led to Integrated Sensor Technologies, Inc. ISTI is an emerging company focused on creating integrated oxygen/OLED sensors. The novel sensors will greatly reduce the expense and size, lessen the energy consumption and ease the process of sensor fabrication, explains Ruth Shinar, CEO of ISTI.

She notes that ISTI's sensor development is in the "exploratory stage," which has been allowed to progress thanks to the assistance in securing research funding provided by ISU's Institute for Physical

Research and Technology. She says IPRT technology commercialization specialists were instrumental in helping ISTI obtain a Small Business Innovative Research grant from the National Institutes of Health.

Sensibly and stylishly simple

Joseph Shinar says the proposed oxygen sensor will be palm-sized or smaller and that the beauty of the device lies in the fact that the sensor will be structurally integrated with its ultrathin light source, an OLED, in a uniquely simple design.

Unlike conventional oxygen sensors that are expensive and sometimes bulky, ISTI's integrated sensors provide a uniquely simple integration approach that could result in very compact devices. Perhaps best of all, the new sensor will be far less expensive, costing approximately $200, due to its essentially disposable modular OLED/sensing element components.

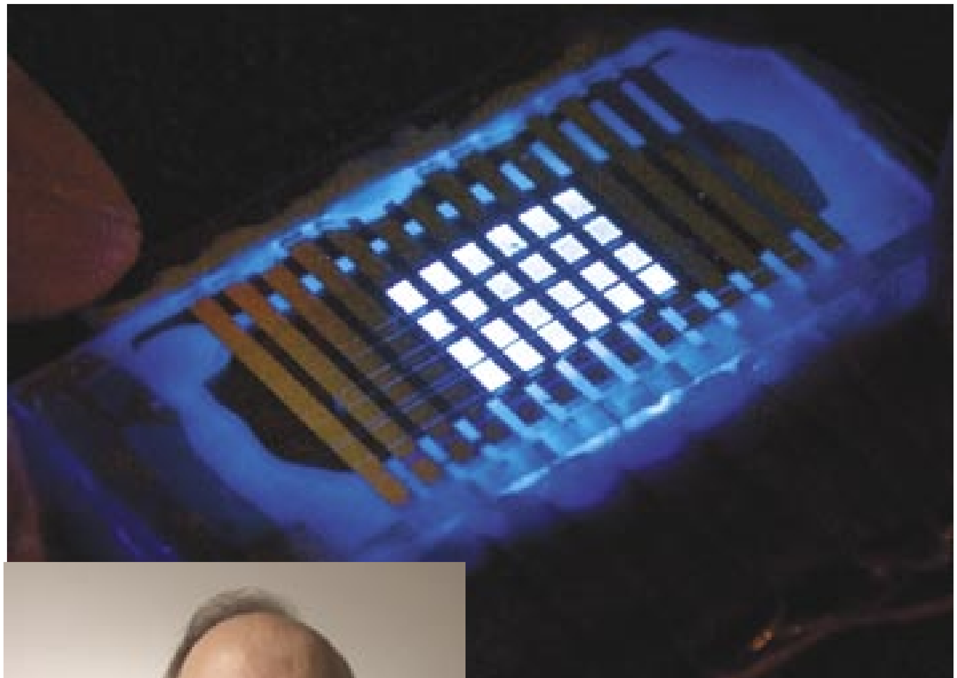
ISTI's novel integrated sensor design may ultimately allow the use of miniaturized sensor arrays with the capability of "front" and "back" luminescence detection, providing a more versatile device with the capability of detecting multiple analytes by utilizing different color, individually addressable, OLED pixels with matching sensing elements.

Out of the lab and into the box

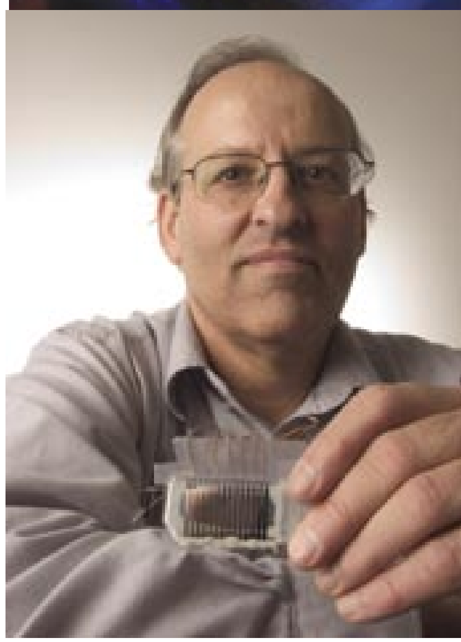
Bhaskar Choudhury, an electrical engineering graduate student working with Microelectronics Research Center Director Vikram Dalal, and Zhaoqun Zhou, a physics graduate student, fabricate the OLEDs for the new oxygen sensors. The Ames Lab Electronics Shop is designing and fabricating a prototype electronics module, power supply and photodetector assemblies – a challenging task.

"It's one thing to demonstrate an oxygen sensor using these OLEDs in the lab, but to assemble a working device, you have to design and build the electronics and put everything in a box and calibrate the whole thing," says Joseph Shinar. "It's a lot of work, not to mention that it needs to compete successfully with existing devices."

Ruth Shinar says the experience of transferring the knowledge gained in the research lab to an actual product has been quite an adventure. She acknowledges IPRT for its strong support in getting Integrated Sensor Technologies, Inc. off to a good start, and Mike Upah, program manager at ISU's Pappajohn Center for Entrepreneurship, for his support. "All involved are strongly focused on the mission of technology transfer," she says.



This brilliant blue organic light-emitting device, or OLED, is integral to a new oxygen sensor that is making its way from basic research at Ames Laboratory to marketable product for the new Ames company, Integrated Sensor Technologies, Inc. The novel sensor technology structurally integrates a photoluminescence-based oxygen sensing element with its OLED light source.



Joseph Shinar has seen his original research on the photophyhsics of luminescent organic thin films and organic light-emitting devices go from bench science to a novel integrated oxygen sensor and a new sensor company.

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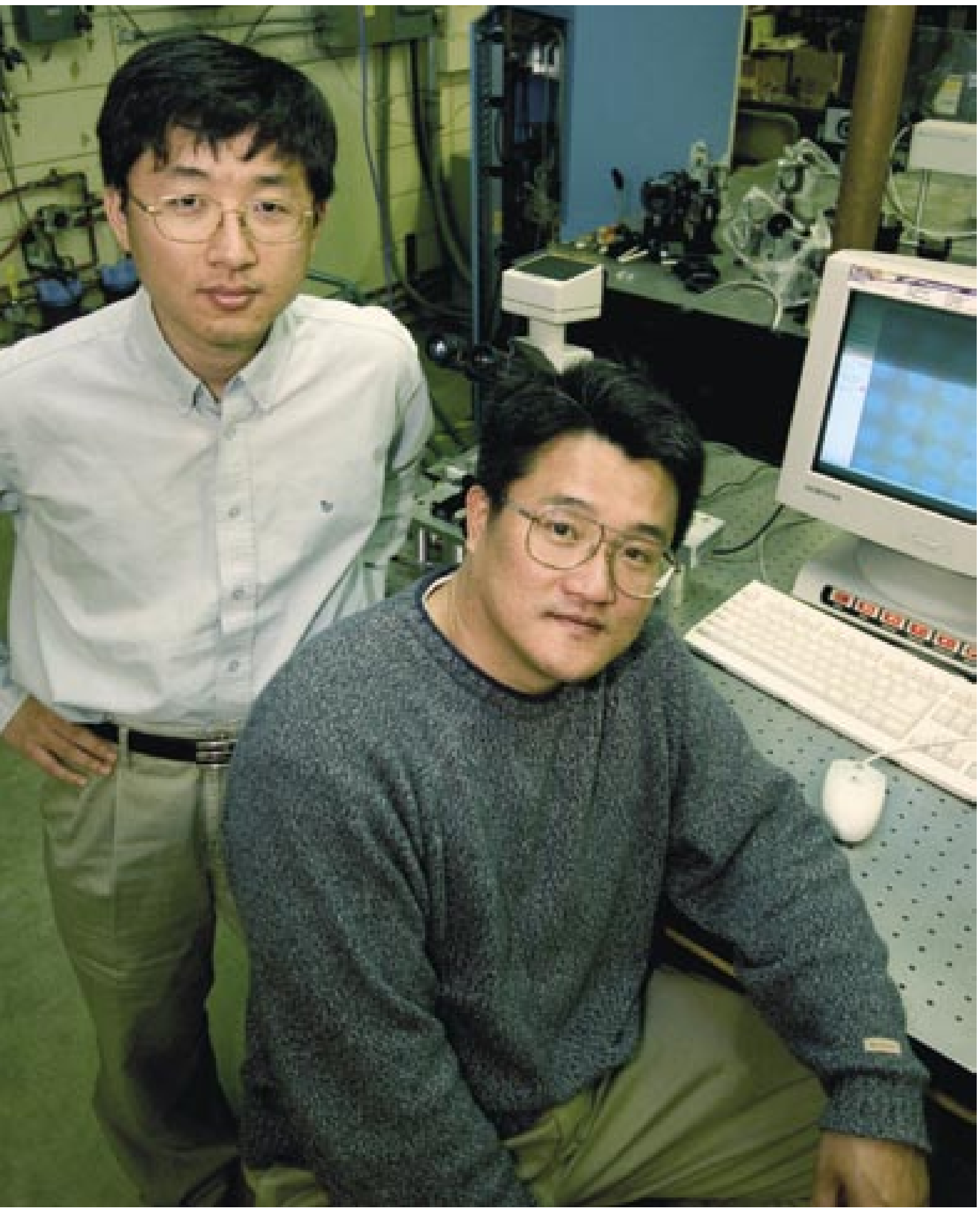
"Tall" Crystals from Tiny Templates

Researchers have modified an old technique to make 3-D multilayered structures

by Saren Johnston



Jae-Hwang Lee (standing) and Chang-Hawn Kim have developed an innovative method based on diffracted moiré fringes for aligning the layers in a photonic crystal.

Hard to hold and hard to handle, like a child in its "terrible twos," light does what it pleases, defying attempts to control its behavior. But while the impulsive actions of toddlers will probably always challenge and test us, scientists are getting better at controlling the spontaneous emission of light.

The ability to trap and manipulate light has been improving steadily since the early 1990s when photonic bandgap crystals and the possibilities they foretold first began to "wow" the scientific community.

Photonic crystals are man-made devices that can be constructed to permit or block the transmission of light of certain frequencies in all directions. This characteristic makes them especially promising for applications within the field of optical communications, where the push is on to create a photonic crystal within a single computer chip.

The research path to that goal is an unbelievably expensive one. But Kai-Ming Ho, an Ames Laboratory senior physicist, and Kristen Constant, an Iowa State University associate professor of materials science and engineering, and their co-workers are easing the way by fabricating 3-D photonic crystal microstructures in the open air, something that has never been done before.

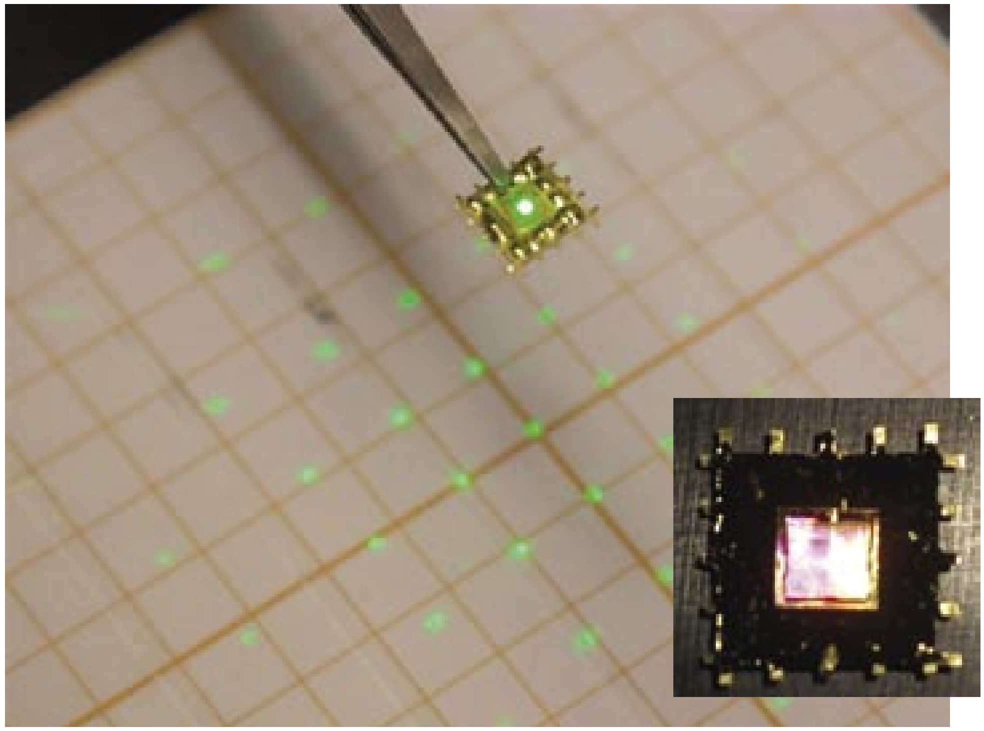
Nothing like it

Achieving a first in the world of novel optical materials, the researchers are making photonic crystals four millimeters square (approximately one-eighth of an inch square) and 12 layers high without benefit of a “clean room” environment or the multimillion dollar equipment traditionally required to create such structures, although multi-domains exist in each crystal and alignment remains a challenge. The fundamental research holds potential for significantly reducing the costs associated with fabricating photonic crystals.

The project is based on Ho’s original 1990 work in which he theoretically demonstrated the existence of the first photonic crystal through his diamond lattice structure design.

That unique design is key to the multilayered photonic crystals that members of Ho’s and Constant’s research groups are making. They have adapted a technique called microtransfer molding to create templates for fabricating the photonic crystals.

“The microtransfer mold technique is not new,” says Ho, who is also an Iowa State University distinguished professor of physics and astronomy. “Modifying it to create multilevel lattice structures at micron- and submicron-length scales – that is the new advance.”



This green laser diffraction pattern of a 4-layer metallic photonic crystal (inset) shows the alignment of a 4-layer PBG crystal that was created by Kai-Ming Ho and Kristen Constant’s research team.

“Slick” work at a small scale

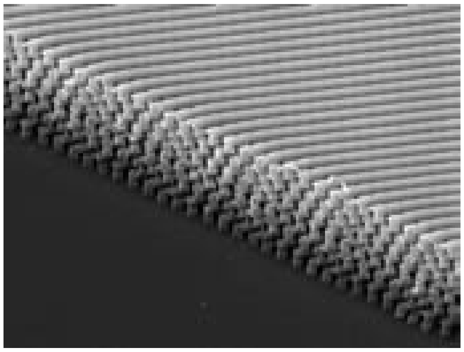
The modified technique involves meticulous work at the micron-scale level. (For size reference, the period at the end of this sentence equals approximately 615 microns.) First, an elastomer mold is created with more than 1,000 microchannels on its surface. The channels are filled with a liquid polymer filler using a manually operated tool. The filler is then solidified by ultraviolet light. Next, the solidified polymer rods in the channels are coated with a second polymer that acts as a glue, bonding the filler to a glass substrate. Once hardened, the elastomer mold is peeled off, leaving a set of parallel polymer rods on the substrate – one layer of the polymer template. By repeating the procedure, in principle, any number of multilayered structures is achievable. To convert the template to a ceramic photonic crystal, the template is over-infiltrated with a titania slurry. The structure is fired to 550 degrees Celsius (1022 F) to remove the template and sinter the titania structure. For metallic photonic crystals, free-standing templates are used with gold sputter deposition.

Stacking microstructures

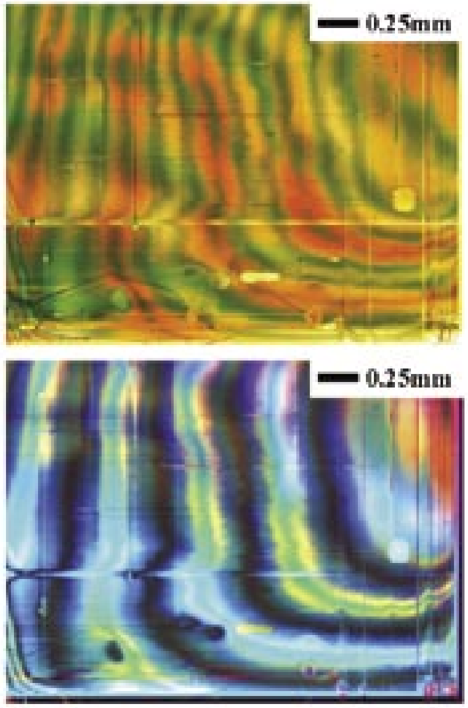
Ho and Constant credit many of the fabrication advances to the unique skills of the young scientists they mentor: postdoctoral fellow Chang-Hwan Kim; current graduate students Jae-Hwang Lee, Yong-Sung Kim, and Ping Kuang; and former graduate student Henry Kang, now at Hewlett Packard in Oregon. They are conquering what is perhaps the biggest challenge – aligning the multiple layers that make up the photonic crystals.

The 1,000 plus rods per layer in a four-millimeter-square photonic crystal are only 2.5 microns apart. “The placement of each rod is so precise,” says Constant. “It’s hard to imagine that we can put something down within a micron or half a micron.”

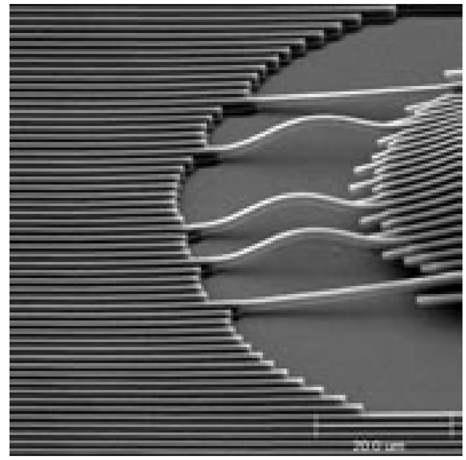
Ho adds, “If you make a mistake in one layer, it will disrupt the next one and spoil the rest of the sample. In order to build multilayers, you



This image of a 12-layer microstructure shows the capability of the modified microtransfer mold technique for fabricating multilayer photonic crystals.



The colorful designs in these two images represent moiré fringes. The top image is conventional moiré fringes, while the bottom image is diffracted moiré fringes. The enhanced contrast provided by the diffracted moiré fringes is essential to the process of aligning the layers in a photonic crystal.



The ability of Ho and Constant's research team to fabricate working photonic crystals outside of a clean room is impressive considering that just a speck of dust can result in defects like the one shown above.

need to get things right successively."

Lee knows the kind of concentration that requires. He has constructed a 12-layer template for a photonic crystal and modestly admits, "I can stack more than this; however it will task my patience!"

To improve the alignment, Lee and Chang-Hwan Kim came up with an ingenious method based on diffracted moiré fringes that has proven indispensable. Ho explains, "Photonic crystals are periodic structures, so any shifts in periodicity will show up over a much larger area. Those shifts are called fringes," he says. "Let's say that the space between rods in a layer is off by one hundredth of the 2.5 microns that separates them. That means that with every 100 rods, there will be a change. The fringes that appear will not be 2.5 microns in size, but 100 times that. The better the alignment, the farther apart those fringes are spaced, so the fringe pattern tells you how good the alignment is."

Constant praises the project's blended research team of physicists and materials engineers. "We've established an expertise with microtransfer molding. It's a niche we can fill that other people aren't doing. When they hear that we're doing this in open air, it really amazes them. It amazes me, too," she admits, "especially when you realize that a speck of dust can disrupt the whole structure."

Ho notes that the care and expertise of the project's team members is overcoming the open-air obstacles. "It's a high-quality, low-cost process – that's the key – and it's achieved by a lot of engineering ingenuity," he says.

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Research funded by:

DOE Office of Basic Energy Sciences
Materials Science and Engineering Division

Science Bowl Scores Big

It's difficult to say who anticipates Ames Laboratory's High School and Middle School Science Bowls more – the volunteers or the student participants. It probably doesn't matter because year after year both the "question-asking" and the "question-answering" teams always seem to have a ball!

The High School Science Bowl saw the hometown team from Ames High School take top honors in the 2005 competition, earning the right to represent the Iowa Region in the Department of Energy's National Science Bowl in Washington, D.C.

After the High School Science Bowl, it was full speed ahead with plans for the Middle School event that included an academic competition and a hydrogen fuel-cell car challenge. Berg Middle School of Newton was victorious in the car challenge, while Central Academy of Des Moines captured first place in the academic competition to receive an all-expenses-paid trip to the National Middle School Science Bowl in Golden, Colo.

Students from Berg Middle School in Newton, Iowa, do a victory dance after winning the Hydrogen Fuel-cell Car Challenge.

From Student to Scientist

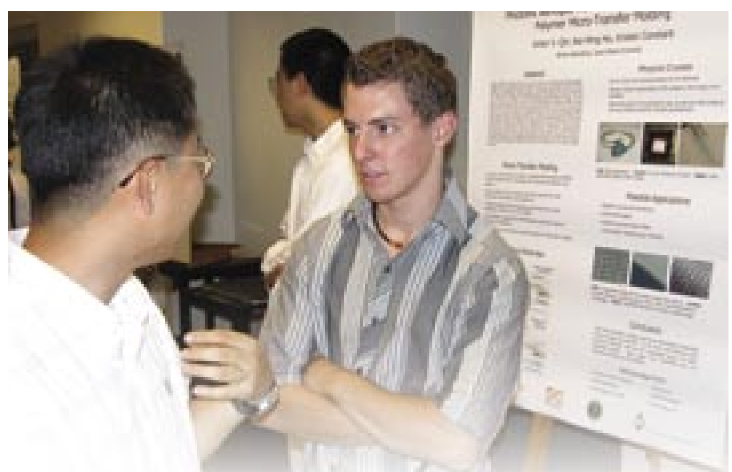
In eight short weeks this summer, 10 undergraduate students from colleges and universities across the country experienced life in a real-world research setting at the Ames Lab. The students were at the Lab as part of the Department of Energy's Science Undergraduate Laboratory Internship, or SULI, program.

The student internships focused on the research the students performed in laboratories under their mentors' guidance. The SULI program culminated with a student research poster session, which was enthusiastically attended by scientists, staff and students.

The following comments are just two of the many positive thoughts expressed by both students and mentors about their experiences in the SULI program.

Iver Anderson, mentor and senior metallurgist – "My experience with the SULI program is colored (brightly) by the extremely high quality of the student, Shamus Cronin, that I worked with this summer. Shamus was willing and able to jump into the project that we designed and was always friendly and positive. I only hope that he got half as much enjoyment out of his experience as my other group members and I received during his stay at Ames Lab. His experimental results were of high (publishable) value, and his careful analysis will help us to develop at least one new manuscript. My only complaint is that the program was too short. Sign me up again!"

Amanda DeVries, SULI student participant – "The SULI program opened my eyes to diversity in the chemistry field as well as basic organic chemistry lab techniques that aren't always taught in the classroom. I worked alongside researchers, something I don't have the opportunity to do at the small school I attend. I am thankful for the brilliant interns, students, and staff I met this summer, and I am thankful for the opportunity the SULI program gave me to further my education in a way I never imagined."



Travis Monk discusses his research poster on photonic bandgap materials during the SULI student poster session.

Searching for the "Holy Grail"

by Kerry Gibson

Praseodymium compounds may serve as models for theorists

In the world of basic research, scientists often look for a material or system that behaves systematically in order to model its behavior. That way, as various factors are changed experimentally, the reactions can be observed and measured. Theorists can use that data to develop complex calculations to explain the behavior.

With a theory in hand, the theorists can further change the variables, perform new calculations and predict the outcomes, while the experimentalists go back to the lab and conduct the same tests under the same prescribed conditions. Finally, they compare the observed results with the predicted outcomes to see if the computational theory holds.

"It's sort of like searching for the Holy Grail," says Ames Laboratory senior metallurgist Bill McCallum. "The ultimate goal would be to choose a combination of elements and simply calculate what compounds will form and what properties those compounds would have. For now, we have to work to find systems that will allow us to continue to push our ability to calculate and understand outcomes."

Interdisciplinary approach

McCallum coordinates an interdisciplinary host of other researchers from the Ames Lab's Materials and Engineering Physics and Condensed Matter Physics programs who are studying one such system, a series of rare earth-nickel-silicon compounds. The group is specifically interested in the magnetic properties exhibited by various praseodymium-nickel-silicon compounds – $Pr_{(n+2)(n+1)}Ni_{n(n-1)+2}Si_{n(n+1)}$, where n = 2, 3, 4 and 5.

"We chose these compounds because they contain well-defined magnetic structures," McCallum says, "and when we made small adjustments in the chemical composition, we expected that the magnetic properties would change in very systematic ways."

The researchers decided to start with samples of the material for the n=3 compound $Pr_{20}Ni_8Si_{12}$ ($Pr_5Ni_2Si_3$). However, problems emerged right away in trying to control the composition of the samples.

"The materials don't form exactly on stoichiometry," McCallum says, "so while we're calling it $Pr_5Ni_2Si_3$ we know that it's actually closer to $Pr_5Ni_{1.85}Si_{3.1}$."

Finding the "good stuff"

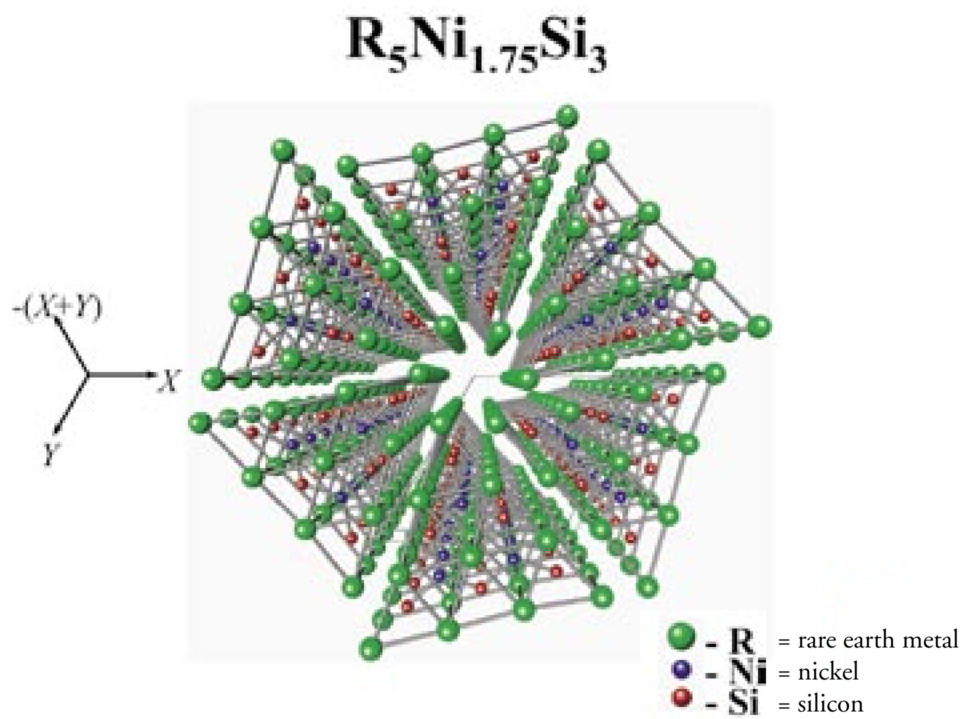
To get around these problems, McCallum relied on physicist Paul Canfield's group to grow single crystals using flux growth methods. Crystals are grown out of a solvent that reduces the melting point of the desired compound.

"Even though the melt was of a different composition than the one we wanted, the correct phase came out of it," McCallum says. "You grow what you want and spin off what you don't want. It's kind of like taking the juice off a roast and after a while the fat congeals, you skim that off and you're left with the good stuff.

"There's a certain amount of guesswork involved so you have to either be lucky or learn a lot about the phase diagrams," McCallum continues, "and we did some of both. We were lucky with our first try and then based on experimental data and thermodynamic calculations we were able to figure out much more detail about the phase diagram."

Although a phase diagram of the praseodymium compound existed, it

(facing page) Ames Lab assistant scientist Dongmei Wu holds a crystalline sample of a praseodymium-nickel-silicon alloy that is the focus of research into how the material's magnetic properties are related to its molecular structure.



This depiction of the molecular structure of the alloy shows the arrangement of trigonal prisms in three neighboring unit cells in the ab-plane.

Ames Lab postdoctoral fellow Yuri Janssen pours molten alloy from a crucible into a centrifuge to separate the desired phase during a flux-growth process.

was apparent that there were significant errors. Impurities in the samples used in the original investigations seem to be the contributing factor, and Ames Lab assistant scientist Sasha Tsokol "put in a tremendous amount of work confirming and correcting the diagrams," McCallum says.

Once they had the "good stuff" to work with, the researchers began taking heat capacity measurements and fairly precise thermal expansion and magnetorestriction measurements. In magnetorestriction, the crystal lattice of the material pulls in when subjected to magnetic fields. However, the praseodymium material exhibited unusual behavior at certain levels.

"We plotted magnetic moment as a function of the temperature in different fields," McCallum explains. "Normally the curves come up in scale, but these have a peculiar peak. So if we fix the temperature and change the field and look at the magnetization, it develops this peculiar transition. It's more pronounced in the smaller (n=2) concentrations and less pronounced in the larger (n=4) ones, but the pattern is the same."

Experimental correlation

Based on the magnetization data for the $Pr_5Ni_2Si_3$, the average magnetic moment – the point at which the material aligns magnetically – was 1.98. Independent neutron diffraction measurements conducted by Anna Llobet-Megias at Los Alamos National Laboratory yielded an average magnetic moment of 2.01. McCallum calls those results an "excellent" correlation. Though neutron diffraction results aren't in yet, similar results are expected for the n=2 ($Pr_6Ni_2Si_3$) and n=4 ($Pr_{15}Ni_7Si_{10}$) compounds.

Even though the crystal structure of the praseodymium materials varies, the experimental findings help paint a consistent picture of what is taking place. And that gives the theorists – Condensed Matter Physics Program Director Bruce Harmon and physicist Min Huang – clearer parameters with which to work.

"If we give them just one structure, there may be various ways to adjust the calculation to fit those results," McCallum says. "But in this material, the various parameters that they can adjust should be the same in each of the three structures. So now we have a much more stringent test because they have to find a set of consistent parameters that give the correct results for all three structures."

While some experimental "clean-up" work remains, the focus now is on developing the theoretical computations to explain what takes place. Those theories will then be tested by further experimentation.

"There really isn't an end result in this," McCallum says. "Hopefully, we can take what we learn here and apply it to other materials."

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Research funded by:

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

INtouch

Physics Fervor

Helping the Department of Energy carry out its mission to lead the U.S. observance of the 2005 World Year of Physics, Ames Laboratory planned and coordinated monthly outreach events that highlighted the seldom-recognized but unquestionably important role of physics in our everyday lives. Event programs included topics for both children and adults. Many of the programs were held at the Ames Public Library in conjunction with the library's summer reading program for young people. Among the Ames Lab offerings were "Physics Sunny-side Up," which highlighted the many things solar energy does on earth, and "Big Chills and Hot Flashes," which amazed both children and adults with the effects of hot and cold on gases, liquids and solids.

A unique program, "Flights of Fancy," took place at Iowa State University's beautiful Reiman Gardens in the exhibit hall near the indoor butterfly wing. The Ames Lab program featured an ISU entomologist and an aerospace engineer who introduced both youngsters and adults to the physics of butterfly flight and the wide array of aerodynamic mechanisms that are involved in the fluttering motion of a butterfly's wings. Visitors then got to make their own colorful, larger-than-life butterflies to take home.

An unplanned but fortunate set of circumstances led to a fascinating WYP evening with Professor E. N. Economou of the Research Center of Crete and department of physics, University of Crete, Greece. Economou was visiting Ames Laboratory senior physicist Costas Soukoulis who requested a lecture from his friend and colleague for Ames Lab's WYP celebration. Economou spoke to a large crowd at ISU's Memorial Union on the significance of two opposing pressures – compressive and expansive – to our world. The balance of those opposing pressures governs the formation of greater and greater structures, from unimaginably small quarks and leptons to larger living structures that include viruses, cells and humans to the ever-greater structures of planets, stars and galaxies, and finally the observable universe.

Unexpectedly, the WYP turned out to be the perfect impetus for getting employees in the mood for Ames Lab's group outing to an Iowa Cubs baseball game. A noon talk, "The Physics of Baseball," by Eli Rosenberg, chair of the ISU physics and astronomy department, included "Seinfeld" clips, cartoons and famous baseball quotes as well as the more detailed physics of the game. The dynamic presentation drew a full house of baseball and physics enthusiasts and succeeded in keeping the less-physics-oriented audience members on track.

During an Ames Laboratory World Year of Physics event at the Ames Public Library, youngsters respond to the directions "be hot" or "freeze" and use a parachute to demonstrate what happens to a helium-filled balloon when dipped in liquid nitrogen.

While creating their own butterfly works of art at an Ames Lab World Year of Physics event on the physics of butterfly flight, youngsters learned that there are as many as six different ways butterflies flap and rotate their wings to stay airborne.

A late summer WYP event planned for the Ames Public Library is the "Totally Toy Workshop." The workshop will provide youngsters with several hands-on opportunities to learn about the physics of various toys, such as Slinkys, yo-yos, and whistles. Future library events that will help round out the 2005 World Year of Physics include programs on the physics of the martial arts and the physics of champagne.

Balancing the Load

Adaptive algorithms ease problem-solving in parallel computing environments

by Saren Johnston

Masha Sosonkina

We tend to shy away from the word "algorithm." For many of us, the term conjures images of lengthy equations and formulas that represent mathematical or computational worlds in which we are not at home. But the fact is that we use algorithms every day. A recipe for making cookies is an algorithm, as are the instructions for building a model airplane or the procedures for knitting an afghan.

An algorithm is a set of steps for solving a specific problem. The steps must be clear-cut and have an obvious stopping point. And although algorithms can be expressed in most any language, they seem to be associated more easily with computer programming languages.

Elegant algorithms

A well-designed algorithm is simple and requires the fewest steps possible to solve the problem, resulting in time- and cost-savings. But creating ingenious algorithms is one of the foremost challenges in programming. Adaptive algorithms facilitate resolution of that challenge. They typically include the ability to modify a running program and balance system resource allocations to react to changing processing conditions.

Most adaptive algorithms operate within the parallel computing environments associated with supercomputers or cluster computers – high-performance computing systems with several processors that can work on different parts of a single problem simultaneously. In a nutshell, adaptive algorithms bring several algorithms together, so to speak, for the solution of the same problem. They also include the mechanisms for choosing the most appropriate algorithm from the available options.

"Today's problems are very complex. They might require many software packages – not all designed for parallel architecture," says Masha Sosonkina, a computational scientist working in the Ames Laboratory's Scalable Computing Lab. "It's very hard to include everything for the solution of those problems in a single software package, so you might want to have some help." That help comes in the form of middleware, which Sosonkina describes as a kind of "middleman" that stands between the computer resources and the algorithm, itself. "Middleware will look at the computer resources and, depending on their current availability, suggest some new algorithm path to the application," she says.

Attach, suggest and optimize

High-performance computing allows scientists to solve very computationally intensive applications, which, Sosonkina notes are sometimes written in older programming languages. "People already have proven codes that work, so we don't want to completely revamp those applications," she says. "What we'd like to have is some lightweight modification – some kind of helper in the middleware to attach itself to these applications and give some suggestions on how to optimize their performance for a given computing environment."

Sosonkina has been working on adaptive algorithms to do just that for the General Atomic and Molecular Electronic Structure System, better known as GAMESS. The computational chemistry code includes a hierarchy of quantum chemistry methods that help solve problems relating to molecules – what they do and why they do it.

With a history that goes back to 1977, GAMESS is what is known as a legacy code. It existed before many recent computer science innovations, so some features of GAMESS have been made parallel from the beginning, and some features have been made parallel after the fact. From the early 1980s to the present, dedicated efforts on the parts of Mark Gordon, Ames Lab program director of Applied Mathematics and Computational Sciences, and Michael Schmidt, an Ames Lab associate scientist, along with many students and postdoctoral fellows, have led to the development of new functionalities for GAMESS and continued parallelization of the code.

Depending on the size and complexity of the molecule under investigation, running GAMESS to compute its electronic structure can make high demands on certain computer resources at various stages of the algorithm, or problem-solving process. According to Sosonkina, the main memory and disk input/output usage are the resources most at risk while GAMESS is executing multiple calculations.

What's needed, Sosonkina explains, is some type of middleware with a system scheduler that can attach to the application, "look" in on the execution of concurrent jobs and then alert the application to the current conditions of the computing environment. This "co-scheduler" then may change the path of the application to adapt it to the chosen environment with the goal of balancing computing resources and making the simultaneous execution of multiple GAMESS calculations more efficient.

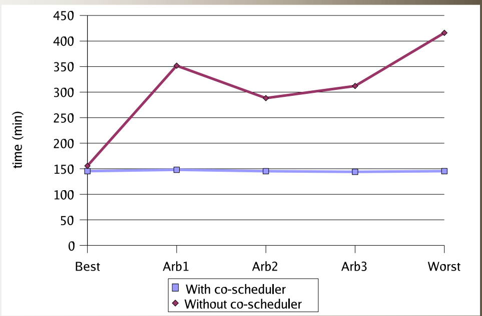
Integrate to monitor

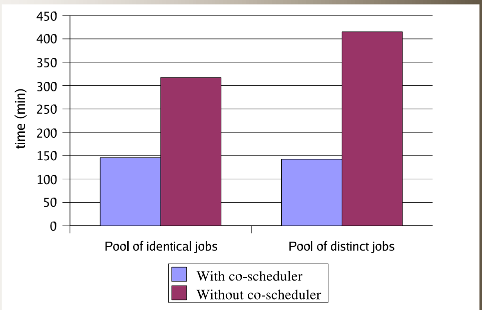
Sosonkina has developed a co-scheduler for GAMESS in collaboration with Nurzhan Ustemirov, an ISU graduate student working with her in the Scalable Computing Lab, and Gordon and Schmidt. Because GAMESS has been around for so long and continues to undergo development, it would be difficult to modify the source code to include a self-scheduler. Instead, Sosonkina and her co-workers are using a middleware tool, Network Information Conveyer and Application Notification, or NICAN, for integration with specific GAMESS algorithms that may have multiple implementations for a given computation. The most appropriate implementation depends on the current state of the computing environment.

The co-scheduler created from integrating NICAN with a GAMESS application separates the process of monitoring computer resources from that of executing the application. It enhances the simultaneous execution of GAMESS jobs while also relaying information about the available main memory to GAMESS. The process is an efficient and timely one due to the monitoring modules within NICAN that watch over different system resources. If a resource reaches a predetermined critical range, NICAN calls up the associated algorithm to "handle" the situation, selecting an appropriate path to execute the GAMESS job. If the critical range for a specific resource is never reached, the adaptive measure is not initiated, and the GAMESS application continues to execute the original job.

Results of experiments conducted on identical as well as different molecules by Sosonkina and her co-workers show that the throughput for GAMESS calculations incorporating adaptive algorithms was dramatically higher compared to the throughput for nonadaptive calculations.

"For the users and developers of high-performance applications, adaptive algorithms coupled with a middleware alleviate the burden of tweaking their programming code depending on changes in the computing environment," says Sosonkina. "The goal is to increase efficiency so computations will finish in reasonable time while maintaining a good utilization of computing resources." To achieve that goal, Sosonkina says there must be a close collaboration between the creators of adaptive algorithms and the application users and developers. "It's very difficult to know the inside of any high-performance software," she adds. "We need teamwork – we require that input to identify the needs of an application."





The top graph shows the time to calculate the structures of 12 identical molecules in the order of different initial algorithmic paths (from Best to Worst, and Arb meaning an arbitrary initial ordering).

The bottom graph represents the average time taken to complete 12 identical and distinct jobs.

Both graphs represent experimental results showing that concurrent GAMESS jobs, in which the adaptations were invoked by NICAN, better utilized the computing resources and, for an arbitrary initial algorithm ordering, resulted in much better performance than the nonadaptive case.

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Photo Gallery

Oxygen Activation Research

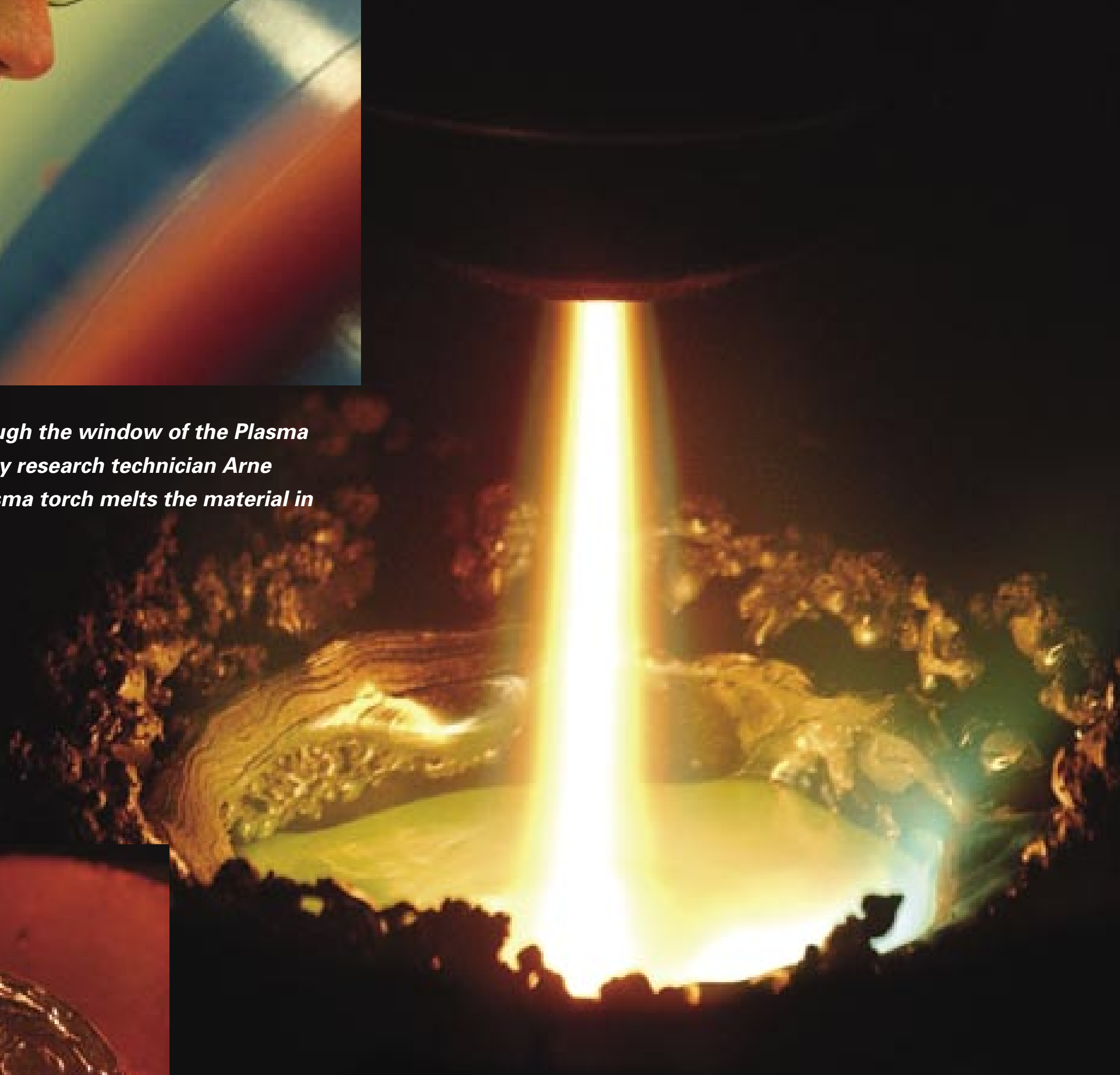
Eyes on the Prize: Kelemu Lemma, an Ames Laboratory postdoctoral fellow, uses a microliter syringe to withdraw a sample of a chromium complex. The procedure is a familiar one in studying the material's reactivity in oxygen activation.

Cool, Clear Water: Water is the solvent in all of the catalysis research led by Ames Laboratory senior chemist Andreja Bakac.

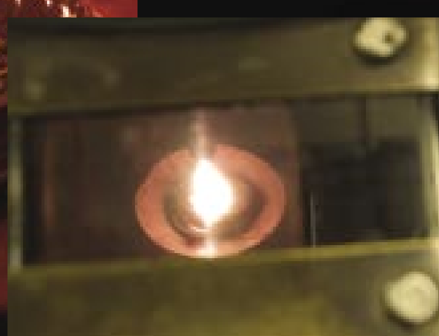
One of a Kind: Dark sample vials are required for light-sensitive metal complexes used in Ames Laboratory's unique research on the catalytic activation of oxygen.

Materials Preparation Center

View to a Melt: Peering through the window of the Plasma Lab Furnace, Ames Laboratory research technician Arne Swanson watches as the plasma torch melts the material in the sample chamber.



A Real Hotshot: The Retech Model 150 Plasma Lab Furnace in Ames Laboratory's Materials Preparation Center generates temperatures well in excess of 10,000 degrees Celsius. The furnace can melt reactive metals and alloys without the need for crucibles to contain them, thus eliminating possible contamination from crucible materials.



Melt Magic: An arc-cast alloy button is placed on a drop-cast mold (left) and melted in an arc melter (right). The resulting alloy melt, among other things, may ultimately be used to produce high-purity single crystals that allow researchers to study and better understand the properties of the material.

Inquiry 2005

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

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