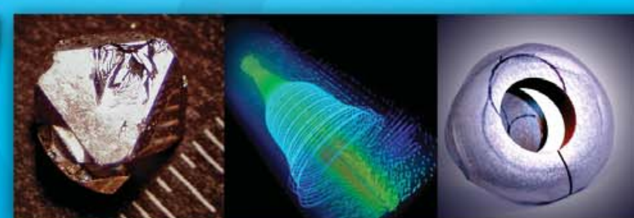
INQUIRY | SPRING 2007

SCIENCE & TECHNOLOGY AT THE AMES LABORATORY

1947

2007



Ames Laboratory

Shaping Science for 60 Years

AMES LABORATORY

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

INQUIRY

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

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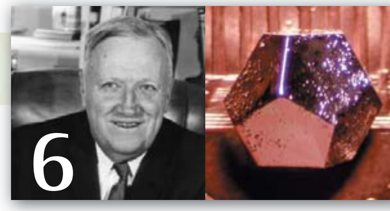
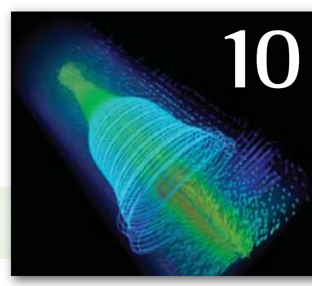




DEPARTMENTS

Cover: *With origins in the Manhattan Project, Ames Laboratory has been shaping science for 60 years.*

From the Director

Welcome to the new, spring issue of *Inquiry*, a publication highlighting the research achievements of Ames Laboratory, a U.S. Department of Energy research facility operated by Iowa State University. In an effort to keep our audiences better informed, *Inquiry* will now be published twice a year instead of just once.

It's just one of many changes taking place at the Laboratory. As I write this letter, a nationwide search has begun to replace Dr. Tom Barton as director, and we look forward to having his permanent replacement in position by late summer. Dr. Barton led the Ames Laboratory for 18 years and leaves behind a commitment to excellence that not only has helped the Laboratory strengthen its status as a world leader in materials research but also has helped expand the Lab's research mission to address new energy-related challenges in materials, chemical, engineering and mathematical sciences, and physics.

Two other major events are impacting the Ames Laboratory in 2007. One is the 60th anniversary of the Laboratory, which we began celebrating on May 17, and that history is celebrated on the cover and the center spread.

The second major announcement is the signing of a new contract between the Department of Energy and Iowa State University for the continued operation of the Ames Laboratory. ISU has been the sole contractor for Ames Lab for the DOE since the Lab's inception in 1947. The new contract, which took effect on Jan. 1, 2007, is a five-year contract worth $150 million. But there are opportunities to extend the contract for up to 20 years based on outstanding performance in our scientific programs. We are confident this extension will be realized.

As exemplified by the research stories in this issue, we have a strong commitment to leading-edge research that responds to the DOE's energy mission. Senior physicist Costas Soukoulis remains a leader in the emerging field of metamaterials. Senior physicist Paul Canfield and scientist Sergey Bud'ko have discovered a family of zinc alloys that can be tuned to take on properties of other materials. And materials scientist Alan Russell and Material Preparation Center Director Larry Jones are using their collective know-how to help develop a cost-effective substitute for palladium to help make hydrogen-fuel technology a reality. The Laboratory remains committed to helping bring appropriate technology advancements to the marketplace to the benefit of the American taxpayer.

In addition, our commitment also extends to doing our part to educate the next generation of scientists and engineers through our symbiotic relationship with our contractor, Iowa State University. As one might imagine, our commitment to quality education and training pays off handsomely for the DOE and our nation through the entrance of a diverse, exceptionally well-trained cadre of scientists and engineers into the labor pool.

Although my time as director of the Ames Laboratory is scheduled to be short, I can assure you that while I'm here our commitment to high-quality research will not wane in the slightest. And I think it goes without saying that our new director will share that commitment as he or she envisions ways in which the Ames Laboratory can grow and prosper in the next 60 years.

Alan Goldman, Interim Director

A Visible Improvement

Pushing the left-handed envelope

BY KERRY GIBSON

FOR THE FIRST TIME EVER, researchers at Ames Laboratory have developed a material with a negative refractive index for visible light. Ames Laboratory senior physicist Costas Soukoulis, working with colleagues in Karlsruhe, Germany, designed a silver-based, mesh-like material that marks the latest advance in the rapidly evolving field of metamaterials.

The advance, detailed in the Jan. 5 issue of *Science*, the Jan. 1 issue of *Optic Letters* and noted in the journal *Nature*, marks a significant step forward from the existing metamaterials that operate in the microwave or far infrared – but still invisible – regions of the spectrum.

Metamaterials, also known as left-handed materials, are exotic, artificially created materials that provide optical properties not found in natural materials. Natural materials refract light, or electromagnetic radiation, to the right of the incident beam at different angles and speeds. However, metamaterials make it possible to refract light to the left, or at a negative angle. This backward-bending characteristic provides scientists the ability to control light, which opens a wide range of potential applications.

"Left-handed materials may one day lead to the development of a type of flat superlens that operates in the visible spectrum," says Soukoulis, who is also an Iowa State University Distinguished Professor of Liberal Arts and Sciences. "Such a lens would offer superior resolution over conventional technology, capturing details much smaller than one wavelength of light to vastly improve imaging for materials or biomedical applications," such as giving researchers the power to see inside a human cell or diagnose disease in a baby still in the womb.

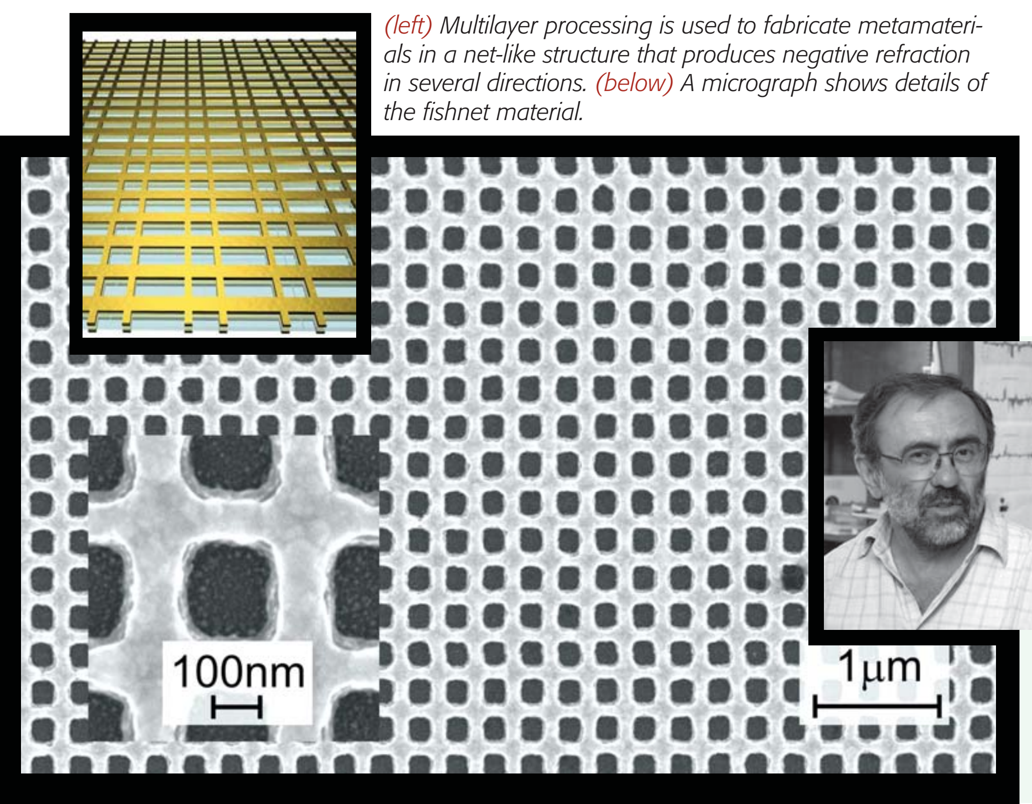
The challenge that Soukoulis and other scientists who work with metamaterials face is to fabricate them so that they refract light at ever smaller wavelengths. The "fishnet" design developed by Soukoulis and produced by nanostructure researchers Stefan Linden and Martin Wegener at the University of Karlsruhe has openings roughly 100 nanometers wide.

"We have fabricated for the first time a negative-index metamaterial with a refractive index of -0.6 at the red end of the visible spectrum (wavelength 780 nm)," says Soukoulis. "This is the smallest wavelength obtained so far."

While the silver used in the fishnet material is more resistant to metal loss when subjected to electromagnetic radiation than gold used in earlier materials, metal loss is a major limiting factor. The difficulties in manufacturing materials at such a small scale also limit the attempts to harness light at ever smaller wavelengths.

"Right now, the materials we can build operate in only one direction," Soukoulis says, "but we've still come a long ways in the six years since negative-index materials were first demonstrated.

"However, for applications to come within reach, several goals need to be achieved," he adds. "We need to reduce losses by using crystalline metals and/or by introducing optically amplifying materials; develop three-dimensional rather than planar structures; create isotropic designs; and find ways of mass producing large-area structures."



(left) Multilayer processing is used to fabricate metamaterials in a net-like structure that produces negative refraction in several directions. (below) A micrograph shows details of the fishnet material.

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Research funded by:
DOE Basic Energy Sciences,
Materials Science and Engineering Division

A single crystal of YFe_2Zn_{20} is shown next to a mm scale. It grows in this shape naturally and has mirrored facets.

The Great Zinc Rethink

Physicists tweak zinc to get model compounds

BY SAREN JOHNSTON

Although ancient alchemists failed to turn base metals like lead into precious ones like gold and silver, one aspect of their misguided efforts survived ... the zest these "sorcerer scientists" exhibited to dramatically alter the properties of a material. However, present-day chemists and solid-state physicists pursue this passion according to scientific protocol, carefully making small changes in the composition of various compounds, especially ones that can be fine-tuned to extremes in behavior. Such is the challenge that entices Ames Laboratory's novel materials group.

Ames Laboratory physicists Paul Canfield and Sergey Bud'ko along with Shuang Jia, a graduate student in Iowa State University's department of physics and astronomy, have discovered a fantastic range of properties in a new family of zinc compounds. Even at over 85 percent zinc, the compounds can be tuned to take on some of the physical properties and behavior of other materials, ranging from copper to more exotic and complex compounds that are on, as Canfield says, "the hairy edge" of becoming magnetic (or even superconducting). Their versatility makes the new zinc compounds ideal for basic research efforts to observe and study the origins of phenomena such as magnetism.

The extraordinary tunability of the RT_2Zn_{20} (R=rare earth, T=transition metal, Zn=zinc) compounds has allowed the Ames researchers to make scores of different compounds with this "one rare earth-two transition metals-twenty zincs" formula. "We can make compounds for up to 10 transition metals, and for each of those we can include between seven and 14 rare earths," says Canfield. "So that's 70 to 140 compounds."

One compound, YFe_2Zn_{20} (Y=yttrium, Fe=iron, Zn=zinc), is even closer to being ferromagnetic than palladium, a nearly ferromagnetic material traditionally studied to better understand magnetism. Canfield says palladium is a "runner-up" in terms of band magnetism – the magnetism of the common metals like iron, cobalt or nickel. These metals become ferromagnetic at such high temperatures that it's difficult to study them in detail, so palladium is the next-best option

"But palladium is a little hard to tune," says Canfield. "For basic research and possible applied materials, you want compounds that allow for the manipulation of their properties. We can tune the rare earth-iron(2)-zinc(20), so we can push these compounds even closer to ferromagnetism and try to understand the consequences."

Canfield, Bud'ko and Jia have tuned the zinc(20) compounds by substituting on the rare earth site, for example, by exchanging yttrium for gadolinium. "Gadolinium makes the compound suddenly go ferromagnetic at an unexpectedly high temperature," says Canfield.

The researchers can also tune the zinc(20) compounds by "playing" with the transition metal site. "By substituting cobalt for iron, we can back this material off," says Canfield, "so we can calm things down a little and see what happens."

The unique tunability of the new zinc(20) compounds is allowing Canfield, Bud'ko and Jia to approach the ferromagnetic transition point from where they hope to push the material to become ferromagnetic at very low temperatures. "If we could do that," says Canfield, "we could actually witness the birth of this type of small-moment ferromagnetism. Instead of just before-and-after pictures, we could watch the whole film."

Working toward that goal, Canfield and Bud'ko stress the importance of being able to draw on the resources available at a U.S. DOE laboratory. "It's important to have design, synthesis and characterization tightly linked," says Canfield. "You need your intrepid band of explorers able to investigate and contribute. Ames Lab has the world's highest purity rare-earth elements, which we need to explore the effects of substitution on the rare-earth site. Also, band structure calculations have been very important in these nearly ferromagnetic materials, so the band structure expertise of our Ames Lab colleague German Samolyuk has been incredibly useful in helping us figure out the next moves."

Q

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Research funded by:
DOE Basic Energy Sciences, Materials Science and Engineering Division

Canfield *Bud'ko* *Jia*

Ames Laboratory

Shaping Science for 60 Years

With roots in the Manhattan Project and the development of a new process for refining uranium, Ames Laboratory has been a leader in the development, synthesis and characterization of new materials throughout its 60-year history. The accomplishments shown here represent just a few of the many scientific contributions that have come from the researchers at Ames Laboratory since its inception on May 17, 1947.

Frank Spedding and Harley Wilhelm led the uranium purification efforts during the Manhattan Project. Spedding later became the Lab's first director.

Frank Spedding

Harley Wilhelm

Art D'Silva, assistant chemist, shows the phosphor image intensifer screen that he and Velmer Fassel, deputy director, developed.

1940

1950

1960

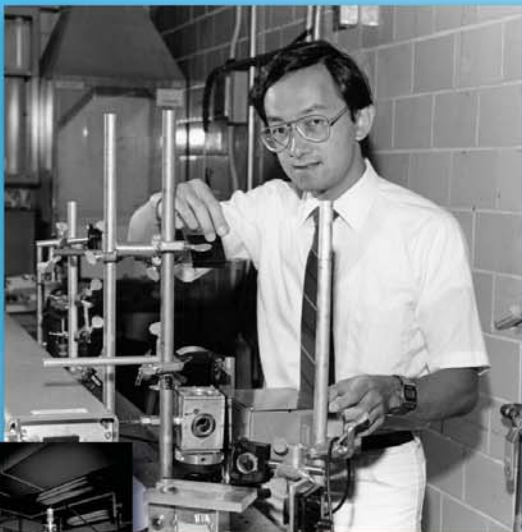
1970

A uranium biscuit produced using a bomb-reduction process discovered by Spedding and Wilhelm.

Ames Lab operated a research reactor from the early 1960s to 1978.

Inductively coupled plasma-atomic emission spectroscopy.

1947 - 2007



Ed Yeung is a multiple R&D 100 award-winner for separation technologies.

Sam Houk adjusts inductively coupled plasma-mass spectrometry equipment used to provide ultratrace analysis for elements and isotopes.

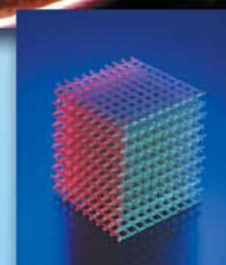
Magnesium-diboride was shown to superconduct at temperatures higher than previously seen.

Ames Lab is a recognized leader in quasicrystal research as well as the growth of single cyrstals.

1980

1990

2000



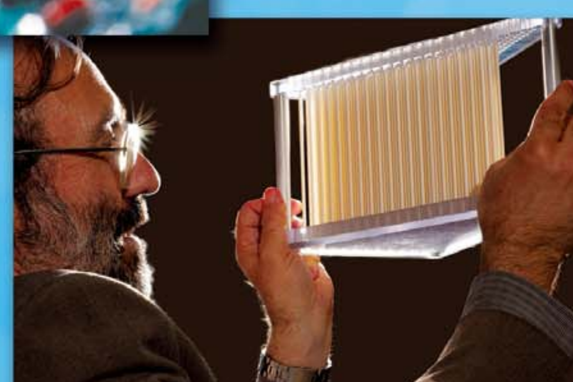
Photonic band-gap crystals offer the ability to control light the way semiconductors control electricity.

Magnetic refrigeration was proven possible using a gadolinium-silicon-germanium alloy developed by Karl Gschneidner and Vitalij Pecharsky.

Lead-free solder developed at Ames Lab is licensed worldwide and has generated more than $10 million in royalties.

Iver Anderson holds a nozzle used in high-pressure gas atomization to produce ultrafine metallic powders.

John McClelland developed an R&D 100 award-winning technology for a photoacoustic cell.



Costas Soukoulis holds a photonic crystal that can negatively refract light.

"Quite an Honor"

Karl Gschneidner named to the National Academy of Engineering

BY KERRY GIBSON

ONE WALL OF KARL GSCHNEIDNER'S SPEDDING Hall office is chock-full of honors and awards the Ames Laboratory senior metallurgist has received throughout his distinguished career. But he'll soon have to make room for the biggest honor of them all – the one that names him as a member of the National Academy of Engineering. Gschneidner was one of 64 American researchers and nine foreign associates inducted into the prestigious Academy earlier this year.

Karl Gschneidner

"It's quite an honor, considering all the competition," he says. "There are a lot of good people out there, so I'm glad we made it!"

The National Academy of Engineering is one branch of the National Academies organization that also includes the National Academy of Sciences, the Institute of Medicine and the National Research Council. Established in 1964, the NAE has a fairly exclusive membership with only 1,945 Americans and 184 foreign associates inducted in its 43-year history.

Academy membership honors those who have made outstanding contributions to "engineering research, practice or education, including, where appropriate, significant contributions to the engineering literature," and to the "pioneering of new and developing fields of technology, making major advancements in traditional fields of engineering or developing/implementing innovative approaches to engineering education."

Gschneidner was specifically cited for "contributions to the science and technology of rare-earth materials," a further acknowledgment of his role as one of the world's foremost authorities in the physical metallurgy and thermal and electrical behaviors of rare-earth materials. An Ames Lab researcher and Iowa State University faculty member since 1963, he became the first director of Ames Lab's Rare-Earth Information Center when it was established in 1966. He has published over 500 papers in the field, and his research in magnetic refrigeration is widely recognized throughout the world.

Gschneidner is also a Fellow of the American Society for Materials International, The Minerals, Metals and Materials Society and the American Physical Society. He is an honorary member of the Materials Research Society of India and The Japan Institute of Metals.

He is the fourth Ames Laboratory researcher named to the National Academy of Engineering and only the sixth overall with ISU ties. He joins Ames Lab's Nondestructive Evaluation Program Director and fellow Iowa State University Anson Marston Distinguished Professor Bruce Thompson, associate researcher Dan Schectman (Materials Chemistry and Biomolecular Materials), and retired researcher Donald Thompson (Nondestructive Evaluation). Senior chemist John Corbett is a member of the National Academy of Sciences.

While he was aware he'd been nominated for the Academy, Gschneidner says his actual election was a surprise. However, he doesn't expect the "fame" to necessarily be followed by fortune.

"People have asked me if this means I'll be getting the big bucks," he says. "Actually, it's going to end up costing me $200 a year for the membership," though he adds with a chuckle that he'll get a discount because of his age. (He turns 77 in November.)

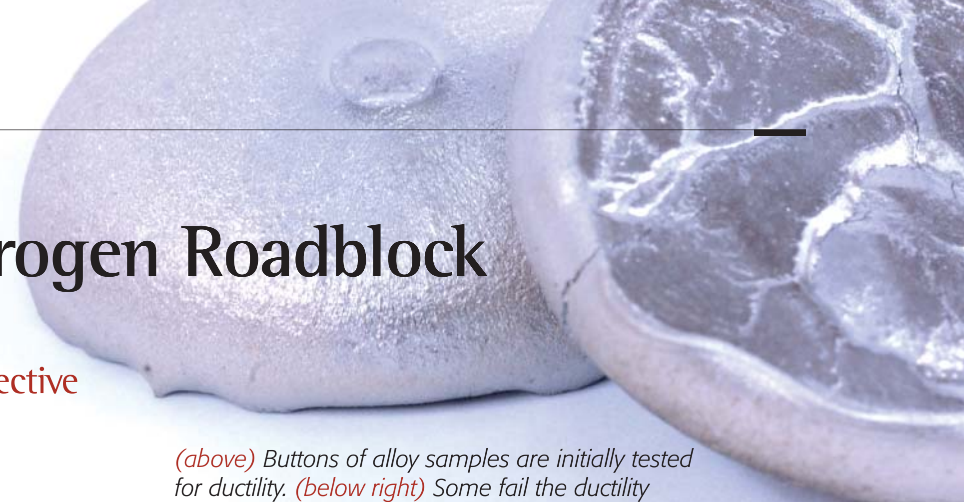
And don't expect him to rest on his laurels. He still maintains a full schedule, splitting his time between the research lab, the library and the lecture circuit.

"I plan to keep doing the same things – looking for new things and trying to figure out what makes them work," he says. "It's what keeps me young."

He also credits those working with him, particularly senior scientists Vitalij Pecharsky and Alan Russell in recent years, for much of his success.

"It's like an orchestra conductor or the manager of a ball team," he explains. "They often get the credit, but without all those talented people around them, they wouldn't get far. I've been fortunate throughout my career to be surrounded by top-notch people and to have a wonderful, supportive and understanding wife."

Q



Removing a Hydrogen Roadblock

Palladium substitute could make hydrogen fuel-cell technology effective

BY KERRY GIBSON

(above) Buttons of alloy samples are initially tested for ductility. (below right) Some fail the ductility test, but those showing promise are rolled and cut for further testing for hydrogen permeability.

AMES LAB RESEARCHERS ALAN RUSSELL AND Larry Jones are employing some modern-day alchemy in an effort to find a material with properties of rare and high-priced palladium. If they're successful, it could remove a major roadblock from the path of hydrogen fuel-cell powered vehicles.

Hydrogen fuel-cell technology sounds almost too good to be true. You combine cheap and plentiful hydrogen and oxygen gas, the fuel cell generates electricity and the by-product is simply water. But if the hydrogen gas contains impurities, such as water vapor or carbon monoxide, it can "gum up" the fuel cell's separation membrane, dropping efficiency or halting the process altogether. Pure hydrogen, however, is hard to come by, and that's where palladium enters the picture.

"Palladium acts like an atomic filter – the hydrogen atoms readily diffuse right through the metal," Russell says. "But palladium is $11,000 a kilogram, and even if you didn't choke at the price, there isn't enough palladium in the entire world to convert the world's automobiles to hydrogen power," Russell says. "So the trick is to find a material with the same properties as palladium that is cheaper and much more readily available."

His use of the word trick isn't a stretch. Not only does the material have to be less expensive and readily available, it has to allow hydrogen to pass through it and be ductile enough to be drawn into long, thin tubes. It also has to resist oxidation, because oxygen and water vapor are commonly present in impure hydrogen. And finally, hydrogen has a nasty habit of making metals brittle, so the metal also has to handle repeated heating and cooling cycles, while loaded with hydrogen, without becoming brittle.

"With so many variables, we don't really have any analytical tools that would let us mathematically predict the ideal composition," Russell says, "so we have to use a Thomas Edison approach – relying on intuition and a fair amount of luck to come up with a combination that works."

The three-year project is being spearheaded by Robert Buxbaum, president of REB Research, a Michigan firm involved in hydrogen filtration and fuel-cell technology. Buxbaum proposed developing 100 different alloys, relying on the expertise of Russell and Jones in the field of metals development to pick the mixtures.

Roughly halfway through the project, about 60 binary alloys have been developed with additional ones in the planning stages. The results have been mixed, but Russell indicated one sample is quite promising, and several others show promise.

"There have been surprises. Some alloys that you would expect to be ductile turn out to be hopelessly brittle, like glass," Russell says. "We also tried a material with 25 percent ruthenium, an element which is notorious for making alloys brittle, but that material turned out to be quite ductile."

Samples produced in Ames are first cold rolled to see if they are ductile. Those showing promise are further tested and shipped to REB Research where they're tested to determine how easily hydrogen will diffuse through the metal. Those showing promise get further testing to see if they can be formed into tubes and how they respond to heating and cooling cycles. But even those materials that are rejected as a palladium substitute may ultimately wind up as useful for other purposes.

Alan Russell

Larry Jones

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Research funded by:
REB Research, from a DOE grant supporting the Hydrogen Fuel Initiative

New research program studies simulation, modeling and decision science

SimCity

Software developed by researchers in the new Simulation, Modeling and Decision Science program allows users to enter a virtual environment that displays velocity information from a data set about the birth of a star.

BY BREEHAN GERLEMAN

ENGINEERS CAN LOOK INSIDE A POWER PLANT, adjust a row of processors and quickly see the results all with a few mouse clicks using virtual engineering tools developed by researchers at Ames Laboratory. Such tools are among software programs developed by the new Ames Lab Simulation, Modeling and Decision Science program designed to help engineers make faster and better design decisions.

Simulation, modeling and decision science researchers create computer applications that convert large 3-D data sets into virtual models that perform just like real-world versions. Engineers view and interact with the models on their computer screens or in a virtual-reality room.

"Simulation, modeling and decision science brings together all the pieces of engineering data, and engineers can actually see what they are doing," says Mark Bryden, Ames Laboratory scientist and Iowa State University associate professor of mechanical engineering, who directs the new program. "They can take a close look at a fan in a virtual engine, make a change to the fan, and then immediately see what happens to the engine's heat-removal capability in the virtual environment."

Trying out engineering plans in the virtual realm leads to sound problem-solving and design in reality.

"We are interested in how engineers can deal with uncertainty in design, and how we can help engineers make good decisions," Bryden says.

Bryden and his team have been studying simulation, modeling and decision science at Ames Lab for several years, and the virtual engineering tools are already in use in DOE projects. Researchers are developing software to model FutureGen, an experimental power plant planned to be the first coal-fueled, near-zero-emissions plant in the world. They also are using the software for turbine- and sensor-modeling research.

Virtual engineering research did not fit into any existing Ames Lab scientific program, so Lab management created the new Simulation, Modeling and Decision Science program. Bryden's work on TBET, a texture-based virtual engineering tool, won an R&D 100 Award in 2006, and the simulation, modeling and decision science field is growing rapidly.

"We have the only virtual engineering software available right now. We want to continue to be leaders in the field and leaders in enabling change in engineering," Bryden says.

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Research funded by:
DOE Office of Fossil Energy

Iowa City Regina Education Center finished third in the Hydrogen Fuel-cell Model Car challenge at the U.S. Department of Energy's National High School Science Bowl®, April 26-30, and collected a check for $1,250 for their efforts. The money won by the Regina team will be used by their school to promote science in the classroom.

"The fuel-cell competition was great," said Josh Modrick, a senior who competed on the Regina team. "It provided a great opportunity to actually 'do' science."

The Regina team finished 18th overall in the 64-team academic competition portion of the National Science Bowl. The team joined more than 300 students from across the United States who competed in the national event in Washington, D.C. Teams made it to the finals by winning Regional Science Bowl competitions held in their home states. Regina won the 17th annual regional competition sponsored by Ames Laboratory and Iowa State University on January 27 at Iowa State.

(From upper left) Members of the Regina team included Phil Ward, Wes Hottel, Vanessa Shiu, Peter Montag and Josh Modrick.

Middle school students got their own crack at Science Bowl fame by competing in the 4th annual Ames Lab/ISU Middle School Regional Science Bowl competition held at ISU on April 13-14. The two-day event consisted of a hydrogen fuel-cell car challenge the first day, followed by the academic competition on the second day. Evans Middle School of Ottumwa fought off many challengers to win the car race. In the academic portion of the event, Central Academy of Des Moines re-established itself as the team to beat, defeating Eleanor Roosevelt Middle School of Dubuque in a highly competitive championship match. This is the third year in the four-year history of the Ames Lab/ISU Middle School Science Bowl that Central Academy has been the victor. Central Academy's Iowa win qualified the team to compete in the National Middle School Science Bowl in Denver, Colo., June 21-24.

Competitors make some last-minute adjustments to their hydrogen fuel-cell car at the start line.

2007 Middle School Science Bowl champions from Central Academy are (seated, left to right) Luchang Wang, Younan Zhu, Alick Feng; and (standing, left to right) Alan Goldman, Ames Lab interim director; Ian Pierson; Kenny Suh and Joyce Johnson (coach).

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AMES LABORATORY

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