FALL DOURN 2007 SCIENCE & TECHNOLOGY AT THE AMES LABORATORY

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INQUIRY

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

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Inquiry is published biannually by the Ames Laboratory Office of Public Affairs. Iowa State University operates the Laboratory for the U.S. Department of Energy under contract DE ACO2 07CH11358. Ames Laboratory shares a close working relationship with Iowa State University's Institute for Physical Research and Technology, a network of scientific research centers.





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Cover: Ames Laboratory's discovery of intricate, foam-like equilibrium patterns (green image) in superconducting lead represents a noteworthy departure from the long-standing Landau model (purple image). (see story on page 8)

From the Director



irst things first! The search committee charged with finding a replacement for former director Dr. Tom Barton brought five finalists to campus in late August and early September. The candidates were put through a two-day interview process that included an open forum for Ames Laboratory

employees and the campus community. Based upon my own conversations with the candidates, I'm sure that Ames Laboratory will continue its 60-year tradition of excellence in science and engineering research.

You'll find stories on a few of those research efforts within the pages of this issue. Physicist Ruslan Prozorov's discovery that the shape of the entire sample determines the pattern topology and overall magnetic behavior of the system is a significant finding that represents a major contribution to the field of superconductivity. Physicist Adam Kaminski uses a technique called angle-resolved photoelectron spectroscopy, ARPES, to learn more about the interactions of electrons because the manner in which they relate to one another determines most properties of solid materials. And as rising oil prices

Welcome to the fall 2007 issue of Inquiry magazine.

have boosted interest in ethanol as a home-grown alternative fuel, analytical chemist Emily Smith is using a technique known as Raman imaging to help select more sustainable crops that can produce more cellulosic ethanol.

Smith's work marks the first joint research effort between Ames Laboratory and Iowa State University's Plant Sciences Institute. When Smith's project was selected for a twoyear grant by the Institute earlier this year, Ames Laboratory provided matching funds from patent royalties generated by other Ames Lab successes, such as Iver Anderson's lead-free solder and Ed Yeung's work in capillary electrophoresis. While we are by far the smallest of the 10 national laboratories operated for the Office of Science in terms of the number of employees and overall budget, we ranked first among those laboratories in 2006 in the amount of licensing income. It's yet another way that the excellent research being done at Ames Laboratory is paying dividends.

With the Laboratory director search coming to a close, I would like to say that it's been my pleasure to serve this Laboratory as interim director for the past eight months. In that brief time, I've come to a greater appreciation of its dedicated staff and the wide range of talent working on projects in a variety of areas. I am also looking forward to handing things off to the new director so that the Laboratory can continue to move forward as it enters its seventh decade of service to science.

Alan Goldman, Interim Director

N THE ATOMIC WORLD, IT'S ALWAYS "CLOUDY." THE NUCLEUS OF EVERY ATOM EXISTS IN A CLOUD OF ELECTRONS.

When atoms are brought together to form a solid, some of these electron clouds "spread" throughout its whole volume. Investigating those clouds and probing the electrons that create them is Adam Kaminski's business. To do so, the Ames Laboratory physicist uses a technique called angleresolved photoelectron spectroscopy, ARPES, to learn more about the interactions of electrons because the manner in which they relate to one another determines most properties of solid materials. And Kaminski is fascinated by metallic solids, especially high-temperature superconductors and the challenge of discovering how they work.

Electrons are very picky. They inhabit only particular energy levels and

Tokyo," says Kaminski. "So, our system is the second-best in the world.

S CBY TSAREN JOHNSTON

"In the photoemission angle-resolved machine, we can map the band structure exactly to study the electrons that control most properties of conductors," Kaminski explains. By shining an ultraviolet light of much higher energy than visible light on the sample, Kaminski can cause some of the electrons to escape the sample. When electrons are ejected from the sample, the principle of conservation of energy of momentum can be applied to find the initial state of an electron before it escaped.

To help clarify the ARPES method, Kaminski compares it to the medical technique of magnetic resonance imaging. "With an MRI machine, physicians in momentum space with ARPES. But we can still see what the bands look like, the states that are occupied and how electrons interact with each other and the rest of the solid."

Kaminski notes that the ARPES technique has evolved tremendously over the last few years. "With the new types of analyzers, we are able to 'see' electronic bands in explicit detail," he says. The ARPES analyzer sorts electrons according to their angles of ejection, which, in turn, provides momentum information. "Now we can get the data in a matter of five minutes with ARPES, where it previously took months," he says. Using ARPES, Kaminski can analyze many kinds of samples to address different types of problems in which electrons play a critical role, the most demanding of which is the effort to explain high-temperature superconductivity.

"Superconductivity is caused by just a very few electrons at the Fermi

"In nature, very few things are perfect, but this particular phenomenon is never more than two electrons share *absolutely perfect*. the same one. In solid materials at low The resistivity is exactly zero.

temperatures, electrons will fill all of the energy states up to the Fermi level, the highest occupied state. Electrons occupying the high energy levels are Kaminski's favorites because they can respond to external stimuli, such as electric field and temperature gradient.

To better study electrons, Kaminski developed and set up Ames Lab's high-precision, laboratory-based ARPES system that provides energy resolution on the order of one millielectron volt, or 1meV. "There is only one place in the world that has better resolution than we do with this machine, and that's in

can use X-rays or gamma rays to image the inside of the body and see organs such as the heart and kidneys. With ARPES, we can see 3-D images of the bands of electrons directly," he says.

Kaminski continues, explaining that the important aspect of the MRI technique for medical diagnostics is spatial resolution. "Electrons don't have a welldefined spatial position," he notes, "but they do have very well-defined momentum. So instead of working in real space like physicians do, we're working

– Adam Kaminski

level - the highest occupied state," says Kaminski. "It's a very rare phase of matter where you have exactly zero electrical resistance" he explains. "In nature, very few things are perfect, but this particular phenomenon is absolutely perfect. The resistivity is exactly zero."

Cuprate compounds are the most prominent high-temperature superconducting materials, and, although

the materials were discovered in 1986, no one has yet been able to explain why they superconduct. "We can easily make high-temperature superconductors in the lab, but we still don't know the mechanism of how they work," says Kaminski.

However, scientists do know some of the things that separate these materials from conventional superconductors. Every superconductor has a superconducting gap, an energy gap that ap-



Ames Laboratory's lab-based ARPES system has a high-precision XYZ manipulator with closed-cycle refrigerator that cools a sample to 10 Kelvin (minus 441.67 degrees Fahrenheit). The system's lens (long horizontal tube) guides electrons into the ARPES analyzer (shiny, hemispherical piece). pears at the superconducting transition temperature where resistance also disappears. But the superconducting gap in a high-temperature superconductor is very unusual – instead of being the same in all directions, it has a particular direction where the gap appears to go to sleep. "It's very different from conventional materials," says Kaminski. "Using the ARPES system in our lab, we can measure the superconducting gap with enormous precision."

Kaminski also uses ARPES to study the pseudogap in cuprates. "In these materials, the properties can be varied, for example, by adding a fraction of oxygen – 10 to 15 percent," he says. "That changes the properties dramatically." At very low oxygen content, the materials display a phenomenon called the pseudogap. It looks almost like the superconducting gap, and it persists to very high temperatures – well above room temperature.

Kaminski notes that there was a lot of excitement surrounding the discovery of the pseudogap in cuprates. "People thought that with this sort of gap you could easily make cuprate samples superconducting at high temperatures," he says. "But what we found is that the pseudogap is actually not related to the superconducting gap. Instead of being a friend, it's actually a foe."

Kaminski says the pseudogap is just one example of the unusual behavior of these materials. "Nobody knows what this pseudogap phase is," he notes. "We've been studying the properties of this phase in relation to superconductivity with our ARPES system. Hopefully the information we get will provide clues to the origin of this phenomenon.



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Research funded by:

DOE Basic Energy Sciences, Materials Science and Engineering Division "These materials are the reason I started studying condensed matter physics," Kaminski admits. "They're so different from anything we've known so far. No classical theory can explain their behavior. We understand them a lot better now, but that's not to say we know how they work. It's probably one of the most complex problems in physics."





The top panel is an image of Fermi surfaces in LuSb (lutetium antimony) samples grown by Ames Lab senior physicist Paul Canfield. The bright intense lines represent states that form Fermi surfaces. These are the electrons that control most of the properties of conducting solids. Below are images of electron bands along two cuts (indicated by lines A and B in the upper panel).

Optimizing Et kerry gibson

Ames Lab chemist Emily Smith stands next to a test plot of switchgrass, one of several crops she's studying to determine viability for use in producing cellulosic ethanol.



Graduate student Kristopher McKee looks through a microscope to position a sample of plant material.

Using Raman imaging to find a better feed stock

ITH HIGH-PRICED GASOLINE FUELING the demand, ethanol production has jumped dramatically, especially in Iowa where 26 ethanol plants are currently in operation with more in the planning or construction stages. While this surge has meant higher prices for corn, it's also meant higher priced corn-fed beef and the many other products made from corn. There's also concern for the land as farmers move from traditional crop rotation to straight corn production and put marginal land back into production.

To address those concerns, producers are looking for other more cost-effective and sustainable crops. Ames Laboratory analytical chemist Emily Smith is looking at a novel way to help them determine what type of plant material offers the best solution, thanks to a grant this spring from Iowa State University's Plant Sciences Institute that was matched by funds from Ames Lab.

Smith is using Raman imaging to study plant cell structure to determine which crops offer the right combination of cell wall composition and degradation to maximize conversion to ethanol. If successful, a simplified version of the test could even be used in the field to determine if plants were at the prime stage for harvest.

"Just like vintners monitor and test the sugar content of their grapes in the field, biofuel producers could potentially use this technology to determine if their crops were at optimal development for conversion to ethanol," says Smith, who is also an ISU assistant professor of chemistry.

The Raman technique Smith uses employs an optical microscope, and specimens are illuminated with a laser beam. As the laser light hits the sample, some of the light is scattered. By analyzing the scattered light with a spectrometer (spectroscope), Smith can easily and quickly determine the chemical makeup of the plant material. A fiber optic bundle placed between the microscope and the spectrometer allows a direct measure of the chemical makeup at any location on the sample being viewed in the microscope.

"This method has several advantages over other analytical techniques," Smith explains. "First, analysis requires very little material, so you can take small samples from a growing plant over time without damaging the plant." Because only very small pieces of plant material are needed and little time is required to prepare samples, multiple samples can be analyzed quickly, making the technique high-throughput. Smith specifically plans to screen the lignin, hemicellulose and cellulose content of biofuel plant stocks, such as switchgrass, *Miscanthus* (a subtropical perennial grass that can grow 13 feet high), corn, and poplar and willow trees. Lignin interferes with enzymatic conversion of polysaccharides to ethanol, so Smith will use the imaging to help select plant stocks that have low lignin content.

"We hope to find out if lignin content changes over time, with different growing conditions, or with different stock material," Smith says, "so we can determine if there is an optimal time to harvest a particular crop."

Plant material for the project will be provided by collaborator Ken Moore, an Iowa State University agronomy professor and expert in biomass crop systems.

While the scope of this project will be used to study biofuel crops, Smith says the technology could also be used to study other plant materials, such as those used for pharmaceuticals.

Smith has been using the Raman imaging technology to study animal and insect proteins and said it wasn't a "big leap" to study plant material.



The two-year Raman imaging project will be carried out by Smith, right, and graduate students Kristopher McKee, center, and Chien-Ju (Cherry) Shih.

"There is obviously a lot of interest in biofuels right now," she explains. "Given the number of good researchers on campus working in this area, it was an easy decision to get involved in this project."

Smith's work is being jointly funded through a two-year grant from ISU's Plant Sciences Institute and by Ames Laboratory through revenues generated by royalties from other research successes. George Kraus, Ames Laboratory's director of Bio-related Initiatives and newly named director of Iowa State's Institute for Physical Research and Technology, called the collaboration a great first step.

"This is a wonderful opportunity to bring the technological expertise of Ames Lab researchers to bear in solving a problem that's a roadblock to moving biofuels to the next level," Kraus says. "We hope to be a partner in similar projects in the future so that other researchers can take advantage of the capabilities that exist within Ames Laboratory."

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Research funded by: Ames Laboratory through royalty revenues ISU Plant Sciences Institute

The New Look of Superconductivity

Equilibrium patterns in superconducting lead: **left**, Prozorov's "soap-foam" pattern; and **right**, the Landau laminar pattern. Both images are obtained at the same temperature and magnetic field. The only difference is how the magnetic field was increased or decreased to reach equilibrium.

IKE THE SURFACE MOTIF OF A BUBBLE BATH, the spatial distribution of a magnetic field penetrating a superconductor can exhibit an intricate, foam-like structure. Physicist Ruslan Prozorov has observed these mystifying, two-dimensional equilibrium patterns in lead samples when the material is in its superconducting state, below 7.2 Kelvin, or minus 446.71 degrees Fahrenheit.

By relating the complex geometry of the equilibrium patterns to the macroscopic physical properties, such as magnetization, Prozorov has shown that the shape of the entire sample determines the pattern topology and overall magnetic behavior of the system. "You can have the same volume and same mass, but if you just change the shape, you get a different type of response from the sample and a different type of geometry of the equilibrium magnetic field patterns," he explains.

Prozorov's discovery of the elaborate patterns in superconducting lead marks a significant departure from the model first proposed by Russian physicist Lev Landau in the 1930s. Landau's model, which assumes a labyrinth

BY SAREN JOHNSTON

or laminar pattern, has been the unchallenged

standard in physics textbooks for 70 years. Now, Prozorov's innovative research has reopened the whole field of equilibrium in type-I superconductors, which had gone dormant because it was considered closed.

Over the years there have been observations of equilibrium patterns in superconductors that differ from the labyrinth model proposed by Landau. However, the unusual patterns were considered to be defects or fluctuations due to imperfections in the material under study. No one bothered to relate the patterns they were observing to macroscopic properties. No one, that is, until Prozorov.

"It all started with an accidental finding," says Prozorov. "I was trying to calibrate a thermometer in my magnetooptical crysostat, so I put in a very clean, stress-free piece of lead. This is an easy way to calibrate because lead becomes superconducting at 7.2 Kelvin, so when I looked at my sample and saw superconductivity, I knew my thermometer was correct."

But something else wasn't correct, at least not textbook correct. When Prozorov applied a sufficiently large magnetic field and looked at the lead sample in the magnetooptics system, he was surprised to see not the Landau labyrinth pattern but, rather, a pattern of two-dimensional tube shapes that he describes as looking like soap foam. "I was shocked because this was totally unexpected," he says. "So now the big question was which pattern represents equilibrium."

Prozorov's experiments showed that, depending on its purity and macroscopic physical shape, the sample under investigation displayed either the soap-foam pattern or the Landau laminar pattern. He knew that samples like disks or slabs that have two parallel surfaces also have a property known as geometric barrier. Only those sample shapes exhibited the Landau pattern, and only when the magnetic field was reduced. However, Prozorov discovered that shapes without two flat surfaces, such as spheres, hemispheres, pyramids and cones, don't exhibit the Landau behavior. "We observed the foam, or tubular, phase in all of these sample shapes, and we don't have the Landau phase at all," he says. "So it's the foam phase that's the equilibrium state of the system. Most of the past studies were done on samples with flat surfaces, that's why people never observed this previously for decreasing magnetic field."

Emphasizing the difficulty involved in creating these lesscommon sample shapes, Prozorov says, "To observe this soap-foam phenomenon, the samples must be very clean and defect-free with a uniformity of crystal structure. We spent a lot of time trying to make lead samples in the shapes of hemispheres, cones and pyramids and finally succeeded. Having access to the materials expertise available at Ames Laboratory has been a tremendous benefit in our efforts," he adds.





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Research funded by:

DOE Office of Basic Energy Sciences, Materials Science and Engineering Division National Science Foundation Alfred P. Sloan Foundation

UPDATE

Extending the Zinc(20) Family

Not long ago physicists Paul Canfield, Sergey Bud'ko and Shuang Jia discovered an exciting family of zinc(20) compounds that can be manipulated to take on the properties and behavior of other materials. (This research is described in "The Great Zinc Rethink," *Inquiry*, spring 2007.) The highly tunable zinc(20) series, RT₂Zn₂₀ (R=rare earth, T=transition metal, Zn=zinc), allows for many model compounds by substituting on either the rare-earth site or the transition metal site.

Now, expanding on that work, the research team has placed ytterbium, Yb, on the rare-earth site, making a half dozen YbT₂Zn₂₀ compounds. "There are clear differences in how electrons in a normal metal like copper and electrons in the YbT₂Zn₂₀ compounds behave," says Canfield. "Ytterbium is a rare-earth element that is a little schizophrenic. It's am-

bivalent, meaning sometimes it will display magnetism, and sometimes it will get rid of the magnetism totally."

By putting ytterbium on the rareearth site in the RT₂Zn₂₀ series, Canfield and his colleagues were able to make compounds that gradually lose their local moment magnetism at low temperatures. This happens, Canfield explains, when the conduction electrons rally around the Yb magnetic moments and collectively screen, or cancel, them out. This collective behavior of the electrons is called a correlated electronic state.

Using the fantastic tunability of the YbT₂Zn₂₀ system, Canfield and his collaborators have been able to double the number of this type of correlated electron systems. "These are materials that have been poorly explored because there have been such a small number of them," he says. "By increasing the number of



A single crystal of $YbT_2 Zn_{20}$

this type of correlated Yb-based compounds, we're able to start identifying systematic trends in their behavior. On top of that, we have five of these six new materials closely enough related that we can start appreciating the significance of subtle nuances in their properties."

Rolls-Royce Acquires License to Use Turbine Blade Coating

Rolls-Royce Corp. has acquired exclusive rights to use a coating invented by Ames Laboratory researchers that helps turbines stand up to the heat in jet engines.

The unique bond coating will be applied to engine turbine blades made of nickel-based superalloys. Those superalloys are designed for strength but need help withstanding metal temperatures approaching 2,100 degrees Fahrenheit inside the hot section of a jet engine, says Ames Lab scientist Brian Gleeson, a coinventor of the coating.

The bond coating, based on a composition comprising platinum, nickel, aluminum and hafnium, improves the durability and reliability of a ceramic thermal barrier that's applied over the bond coat, says Daniel Sordelet, a senior scientist and group leader for the Ames Laboratory and a co-inventor of the technology, which won a prestigious R&D 100 Award in 2005.

Dr. William J. Brindley, the chief technologist for Rolls-Royce Corp., says, "This new coating offers excellent oxidation resistance. It's a new concept in coatings and a real step forward in understanding how and why coatings work. The technology also represents a remarkably quick transition from fundamental science to practical application."

Rolls-Royce, a world-wide provider of power systems for use in aerospace, marine and energy applications, will have an exclusive license to commercialize the inventions. Patents



Daniel Sordelet and Brian Gleeson

are pending for the inventions, and the term of the license agreement is for the life of any patents. The license has the potential to be an important source of revenue for the Iowa State University Research Foundation.

2006-2007 AWARDS



Mark Gordon • IBM Faculty Award



Rodney Fox • ISU Award for Outstanding Achievement in Research



Robert Angelici ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry



Richard Larock ISU Distinguished Professor of Liberal Arts and Sciences



Mei Hong • ISU Award for Mid-Career Achievement in Research



Sam Houk • Fellow, Society for Applied Spectroscopy

 ISU Margaret Ellen White Graduate Faculty Award



Edward S. Yeung • Fellow, Society for Applied Spectroscopy



Condensed Matter Physics

Alan Goldman • ISU Distinguished Professor in Liberal Arts and Sciences



Marshal Luban Doctor Rerum Naturalium Honoris Causa, Universität Osnabrück



Jöerg Schmalian • Fellow, American Physical Society • ISU Award for Mid-Career Achievement in Research



John D. Corbett • F. Albert Cotton Award in Synthetic Inorganic Chemistry, American Chemical Society



Big 12 Conference
"Rising Star" Innovator

• ISU Award for Mid-Career Achievement in Research







R. Bruce Thompson • Research Award for Sustained Excellence, American Society for Nondestructive Testing's Research Council



Barbara Lograsso SULI Outstanding Mentor Award





Karl A. Gschneidner, Jr Member, National Academy of Engineering Acta Materialia Gold Medal

EDUCATION

Ames Laboratory's Science Undergraduate Laboratory Internship program concluded its third year in 2007. The 10-week SULI program ended with a poster session that provided the 11 student participants the opportunity to share final results of their work with Ames Lab and Iowa State University scientists, students and staff.

This year's SULI students were from colleges and universities in 10 states: the University of California, Berkeley; Northwestern University (Illinois); Pennsylvania State University; Brigham Young University (Idaho); Carleton College (Minnesota); Virginia Tech; the Missouri Academy of Math, Science and Computing; Albion College (Michigan); Manchester College (Indiana); and Grinnell College and Central College (Iowa). Each student was matched with a mentor, either from the Laboratory or ISU, and spent time in research laboratories, where they worked on proj-

Nine creative and motivated middle school teachers from Minnesota, South Dakota, Kansas and Iowa descended on the Ames Laboratory and ISU for four weeks this summer as part of the Lab's newly created DOE Academies Creating Teacher Scientists, or ACTS, program. The four-week session had the students involved in a variety of activities, from training, lectures and workshops presented by Ames Laboratory scientists and staff to visits to research laboratories and field stations for observations. Teachers also conducted their own small research projects to investigate topics in environmental physics, chemistry and earth science.

The goal of the ACTS program is to give participating teachers the skills to develop exciting and innovative science programs in their schools that will encourage students to pursue careers in science and math. Teachers make a three-year commitment to Ames Lab's DOE ACTS program, which means we ects that resulted in either a research paper or PowerPoint presentation.

"My career goals have been confirmed," says SULI student Thomas Brenner. "I've been considering an academic career and this internship allowed me to verify that I do enjoy research."



Tim Pica, (left) an undergraduate from the University of California, Berkeley, works with Lijun Wang, a researcher in Ames Laboratory's Materials Chemistry and Biomolecular Materials program.

can look forward to seeing them again in the summers of 2008 and 2009.

One teacher says this about the

program, "I have developed a better understanding of scientific inquiry both as a scientist and as a teacher."



ACTS participants Laura Cady (left), a sixth-grade teacher from Clarence, Iowa, and Sharon Andrews (right), fifth-grade teacher from Sioux Falls, S.D., adjust equipment on the roof of the Science II building on the ISU campus as part of their research project measuring solar radiation.



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