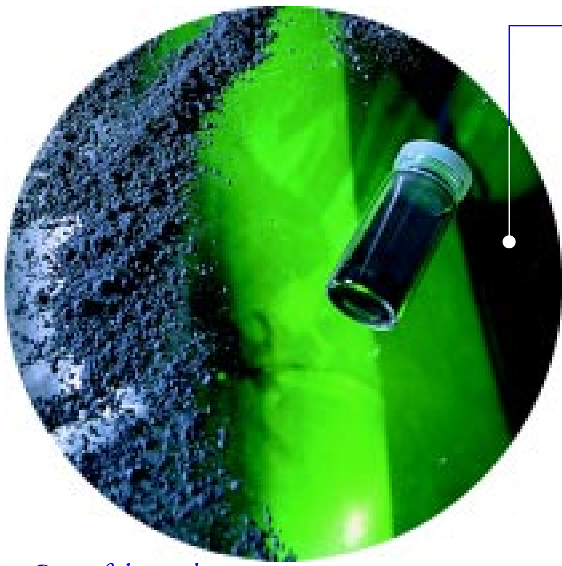
Inquiry

Features

R&D 100 1998 AWARD WINNER



Powerful powder

Cool cloud studies

Letter from the Director

The journey to unravel the secrets of science is a fascinating, yet challenging quest. And as they have for more than five decades, Ames Laboratory scientists continue to eagerly challenge any and all limitations, finding solutions where roadblocks existed in the past.

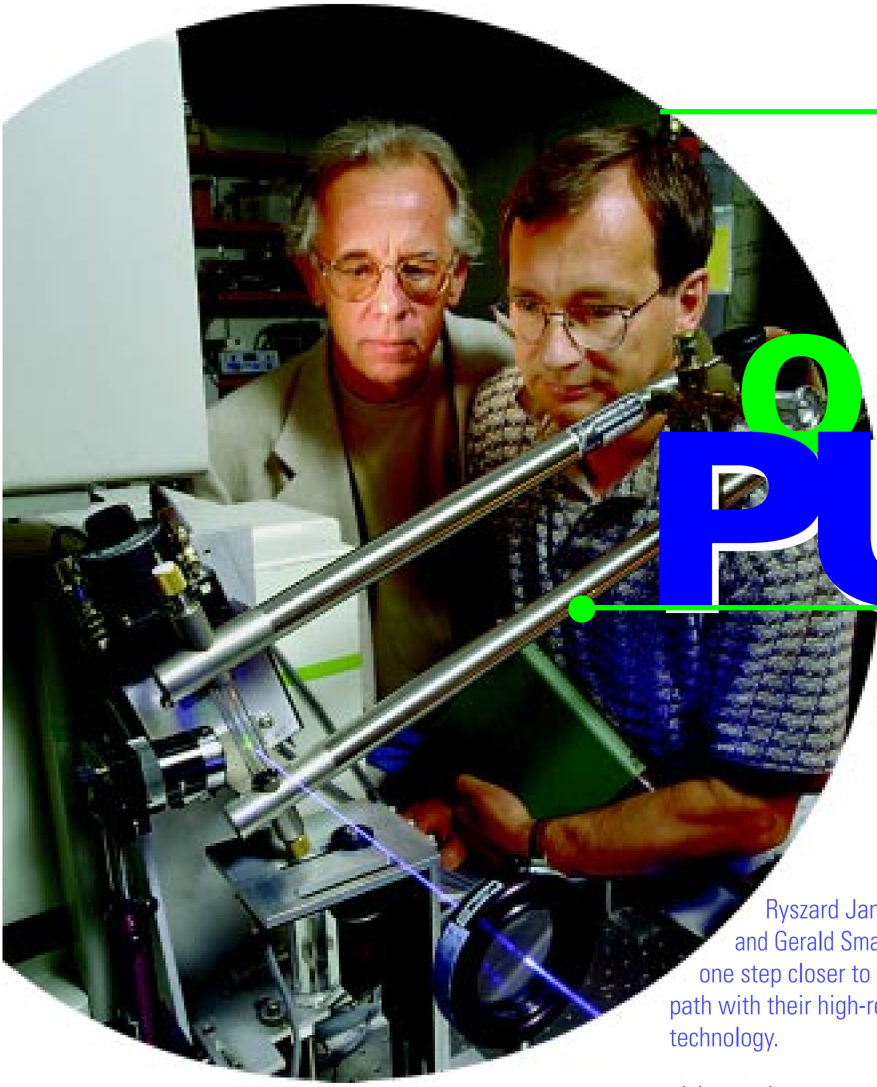
Ames Laboratory conducts its research as one of the U.S. Department of Energy's national laboratories. Well equipped to pursue the challenges that confront our nation and world in energy research, Lab scientists this year investigated scientific challenges that were diverse in scope, not only in terms of area of endeavor but also locale. Here at home, two of our scientists conducted research to help advance the understanding of an individual's risk of getting cancer from chemical pollutants. Their important discoveries netted the two a prestigious R&D 100 Award. Venturing far away from the familiar setting of Iowa, another of our scientists boarded an icebreaker in the far reaches of our planet, the Arctic Ocean, to conduct research that may help unlock the secrets of how clouds affect our global climate.

These fascinating research efforts are just two of the scientific highlights included in this issue of *Inquiry*. I invite you to turn the page and witness the myriad ways in which our scientists reach beyond traditional boundaries to produce good science that ultimately may enrich the lives of the American public.

Tom Barton

GIVING CANCER THE ONE-TWO PUNCH!

by Saren Johnston



Ryszard Jankowiak (foreground) and Gerald Small may have brought us one step closer to uncovering cancer's path with their high-resolution CE-FLNS technology.

They surround us. There's no way we can completely escape them. But if we can learn more about the damage they do to our DNA, we might be able to combat them.

Cancer-producing pollutants, such as those found in cigarette smoke, automobile exhaust fumes and power plant emissions, invade our bodies every day. Over time, the onslaught can create internal havoc as these carcinogens mix with our cellular DNA, the macromolecule that carries our genetic code of life. The chemistry that takes place causes DNA damage and produces byproducts known as DNA adducts, which can lead to mutations. If scientists can identify these byproducts, they may be able to discover which ones lead to cancer.

Searching for needles in haystacks

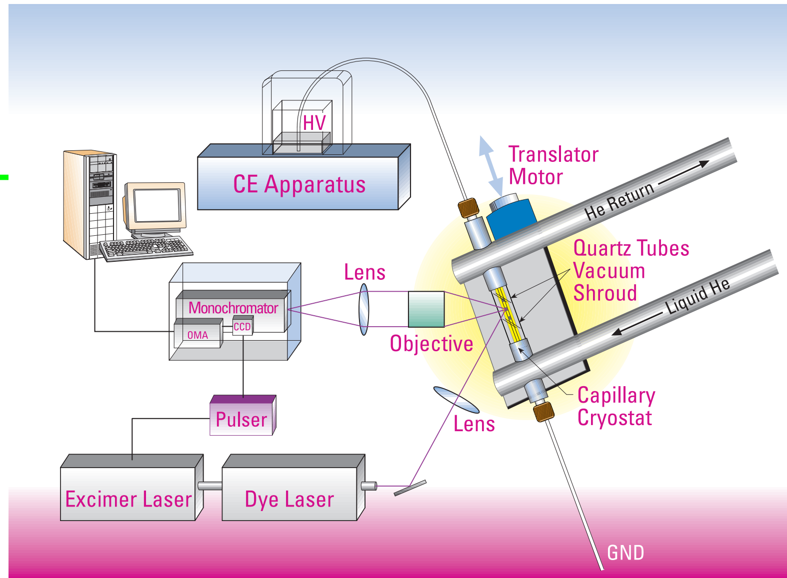
Looking for specific DNA adducts may sound like an uncomplicated plan, but if you're the person doing the searching, you know just how frustrating it can be. Identifying structurally similar cancer-causing compounds and closely related DNA adducts can be a chemical analysis nightmare. A complex biomolecular mixture, such as urine, can contain almost a thousand different compounds. And it can become extremely exacting trying to identify the seven or eight metabolites of interest from the hundreds of others.

Hoping to ease this predicament, Ryszard Jankowiak, scientist, and Gerald Small, senior chemist, combined two well-established analytical methods to create an innovative, on-line technique called capillary electrophoresis – fluorescence line-narrowing spectroscopy (CE-FLNS).

"The marriage of capillary electrophoresis (CE) and fluorescence line-narrowing spectroscopy (FLNS) is an exciting addition to the rapidly evolving field concerned with selective detection methods that can provide the information necessary to distinguish between structurally similar molecular compounds," says Jankowiak.

The power behind the punch

The novel CE-FLNS combination can provide more detailed information on complex biomolecular samples than either CE or FLNS can do on its own. CE-FLNS first takes advantage of the ability of CE to separate minute amounts of closely related biological analytes, or compounds. The second half of the technology combination, FLNS, is a high-resolution, fluorescence-based detection method that was per-



The success of CE-FLNS is due to the design of the compact and fast-cooling capillary cryostat that unites two established analytical techniques, allowing superior identification and characterization of structurally similar compounds.

"It's on-line with minute

fected at Ames Lab for analytical purposes. FLNS makes its contribution to resolving the "molecular identity crisis" by characterizing the CE-separated molecular samples. The process differentiates structurally related analytes by laser exciting them to fluoresce and emit fluorescence line-narrowed spectra, which can be collected and measured.

The power of CE-FLNS was demonstrated in work with the Eppley Institute for Research in Cancer and Allied Diseases at the University of Nebraska Medical Center. The research led to the discovery of a new pathway that chemical carcinogens take for their attack on DNA. "But CE-FLNS makes such research easier and misidentification of analytes far less likely," notes Jankowiak. "Its on-line capability is especially important when dealing with minute quantities of biological materials."

Michael Gross, professor of chemistry and medicine at Washington University in St. Louis, has collaborated with Jankowiak and Small on research to detect and identify trace amounts of pieces of DNA that have been modified by carcinogens. He expresses high regard for the capabilities of the CE-FLNS system. "I watched with interest the design, assembly and successful testing of the prototype CE-FLNS system, and I know first-hand that it has played a vital role in detecting modified DNA," he says. "The new CE-FLNS methodology for on-line structural characterization should significantly enhance the potential of high-resolution spectroscopy, which has already been shown to be the most powerful method to analyze DNA adducts derived from polycyclic aromatic hydrocarbons." (Polycyclic aromatic hydrocarbons make up a potent class of chemical carcinogens.)

Remarkable regulator

Fundamental to the CE-FLNS technique is Jankowiak's and Small's design of a compact and reliable capillary cryostat that regulates and maintains the constant low temperature required for FLNS characterization. The uniquely designed cryostat consists of a double-walled quartz cell that encloses the capillary (a tube with a very small diameter) housing the CE-separated analytes. The capillary cryostat is the critical link that unites the CE and FLNS techniques. Gases and vapors are removed from the outer portion of the cryostat, and inlet and return lines introduce and circulate cryogenic liquids, either liquid nitrogen or liquid helium.

Liquid nitrogen is used to cool analytes to 77 K (-321 F) when low-resolution spectroscopy is sufficient for identification purposes. But when high-resolution spectroscopy is required, liquid helium is used to cool the capillary and CE-separated analytes to 4.2 K (-452 F) in less than one minute. The frozen and stationary analytes can then be sequentially characterized, or "fingerprinted," by FLNS as the capillary cryostat with the enclosed capillary moves automatically along a transmission stage and passes through the laser-excitation region.

More to come for the combo

Although Jankowiak and Small have used CE-FLNS primarily for research on DNA damage from chemical carcinogens, they'll tell you there's definitely more in store for the unique technology combination. Potential applications include other areas of biological research, as well as forensic science.

"Our technology has applicability well beyond just the problem of cancer," says Small. "It could be

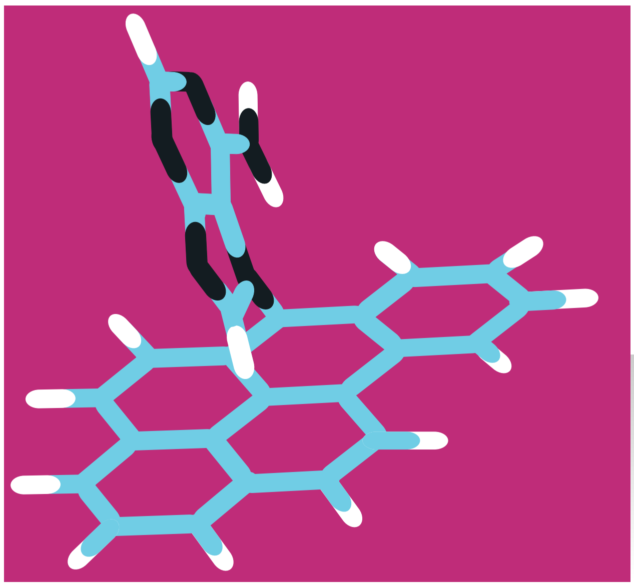
capability is especially important when dealing quantities of biological materials."

used for virtually any biological problem where one has to deal with and unravel complex biological mixtures. We haven't even begun to explore all of the pos-sibilities yet."

The CE-FLNS technology is already being investigated by several companies, and Jankowiak and Small hope to have it licensed and on the market in three years. While all this activity is taking place, the two researchers are simultaneously looking at ways to enhance the capabilities of CE-FLNS.

"We'd like to do a second-generation cryostat and then improve the collection optics to give us more sensitivity," says Small. "At the present time, the capillary cryostat moves only in the direction of its axis. We'd like to put a three-dimensional, or x-y-z, transmission mode in there, too, so it makes it very easy to align the capillary."

But perhaps it is Jankowiak's and Small's fundamental idea and method of pairing two exceptional analytical techniques that will allow them to best improve upon and expand their efforts in on-line characterization of structurally similar compounds. "The versatility of our basic concept can be increased by coupling FLNS with as many different separation techniques as possible," says Jankowiak.◆



This is a calculated structure of a DNA adduct that the CE-FLNS instrumentation was able to identify in the urine of a test group of smokers. The study was done in collaboration with Dr. George Casale of the Eppley Institute for Research in Cancer in Omaha, NE.

For more information:

Ryszard Jankowiak, (515) 294-4394
jankowiak@ameslab.gov

Gerald Small, (515) 294-3859
gsmall@ameslab.gov

Current research funded by:
DOE Biological & Environmental Research Office

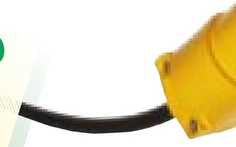
R&D 100 1998 AWARD WINNER

Ryszard Jankowiak and Gerald Small received a 1998 R&D 100 Award for their novel CE-FLNS technology. Their award brings to 13 the number of such prestigious awards Ames Laboratory has earned since 1984.

The R&D 100 Awards Program, now in its 36th year, honors the top 100 products of technological significance that were marketed or licensed during the previous calendar year.

Power to the People

by Susan Dieterle



An electric car whirs along the street as the driver heads home from work. Instead of the noxious fumes emitted by gasoline-powered cars, this vehicle's exhaust consists of little more than water. As the power gets low, the driver pulls into a station where a technician removes the spent fuel container and replaces it with a fresh one.

The driver grabs her cellular phone to let her family know she's on her way. This phone battery lasts longer than the older style and doesn't contain the toxic elements used in earlier batteries. The same is true of the rechargeable batteries in the power tools and electronics at her home.

If you think a scenario such as this won't unfold during your lifetime, think again. Scientists and manufacturers throughout the world are elbows-deep in efforts to develop new types of rechargeable batteries and fuel cells that are powerful, inexpensive and environmentally safe.

Part of this effort involves researchers at Ames Laboratory: Vitalij Pecharsky, scientist; Iver Anderson, director of the Metallurgy and Ceramics Program; and Jim Foley, associate metallurgist. Along with colleagues at four other institutions, they are developing a new class of hydrogen-storage materials for rechargeable batteries and fuel cells. They hope their work will help make cleaner, safer battery power possible – soon.

"Successful completion of our project can really affect the everyday lives of our children and future generations who will place ever-increasing reliance on electrically powered appliances, electronic devices and even electric cars that use the clean, quiet, portable power from batteries or fuel cells," says Anderson, who is also an adjunct professor of materials science and engineering at Iowa State University (ISU).

Hydrogen's appeal

The goal of the \$8.2-million, three-year project is to develop a new class of magnesium-based alloys that can reversibly store and release hydrogen. In addition to Ames Laboratory, the other participants are Ovonic Battery Co., Crucible Research, Oak Ridge National Laboratory and the Colorado School of Mines.

Hydrogen is an appealing fuel choice because it is a clean, abundant, endless source of energy. When it burns in Earth's oxygen atmosphere, it produces water, which can then be broken back down into hydrogen and oxygen.

"Hydrogen is an almost ideal fuel," says Pecharsky, who is also an associate professor of materials science and engineering at ISU.

But using it presents a few difficulties. To be used as a liquid, hydrogen would have to be maintained at 20 degrees above absolute zero, requiring costly cryogenic equipment. It also can be stored as a compressed gas, but this creates an explosive hazard and would involve heavy, bulky storage tanks. The most attractive and safest option involves using certain types of metals and alloys that form unstable hydrides that are capable of absorbing hydrogen in a solid crystalline form and then releasing it when heated.

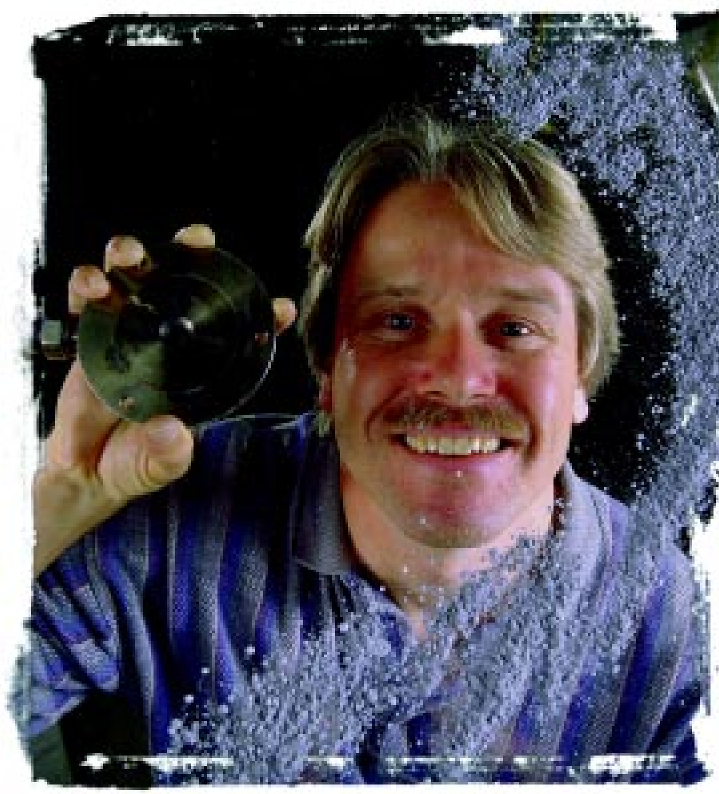
"By using the metal hydrides, you are not stuck with cryogenic equipment, you are not stuck with high pressure," Pecharsky says. "Instead, you have hydrogen trapped inside the metal matrix, which is very safe."

Foley is among those who believe that metal-hydride batteries will be the batteries of choice in the future. "Current and future metal-hydride batteries are considered 'green,' or environmentally friendly, because they don't contain any heavy metals, such as lead or cadmium, that can pollute groundwater," he says.

Some products, such as cellular phones and power tools, already use metal-hydride batteries. Nickel is a basic component in most of the current hydrogen-storage materials. Other common alloy components are rare earths, zirconium and titanium.

When a rechargeable nickel metal-hydride battery goes through the charging process, hydrogen ions from the electrolyzed water present in the battery are reduced and turned into hydrogen gas, which is absorbed by a cathode made of the metal-hydride material. When the process is reversed, the hydrogen oxidizes and reunites with the oxygen, forming water and producing an electrical current in the battery.

In a fuel cell for an electric car, hydrogen is drawn from the metal-hydride material and then chemically combined with oxygen from the air. This reaction takes place within the fuel cell and generates electricity to power the car.



The HPGA nozzle developed by Iver Anderson helps produce ultrafine metal-powder particles with uniform, spherical shapes.

Hopes for magnesium

So, with all of the advantages offered by metal-hydride batteries, why is it difficult to find them on the market right now? Mostly because they are too heavy and too expensive. Current metal-hydride alloys absorb only about 1 to 1.5 percent hydrogen by weight, meaning that storing 1 kilogram of hydrogen requires 99 kilograms of metal-hydride material. They also contain costly elements, such as zirconium, which are sometimes in short supply.

In the search for an abundant raw material that is lightweight, inexpensive and stores more hydrogen, project participants have turned to magnesium. Pure magnesium meets all of the criteria and stores about 6.5 percent hydrogen by weight. "If you think about the commercial applications of magnesium-based alloys, the potential is almost limitless – it's huge," Pecharsky says.

Magnesium has one drawback. It must be heated to 500-600 C (about 1000 F) before it will release the stored hydrogen. But project participants believe they can solve that problem by modifying the magnesium with other elements.

Developing the new magnesium alloys will be the responsibility of Ovonic Battery, a world leader in metal-hydride batteries, with metallurgical assistance from Ames Lab. "The Ames Laboratory is the leading laboratory in the metallurgy field," says Rosa Chiang Young, vice president of advanced materials development for Ovonic Battery. "We need the expertise and all of the experience from Ames Lab to help design this material and really make the program move forward."

Oak Ridge National Laboratory will research different forms in which the alloy can be used. Crucible Research, a company with expertise in powder metallurgy, will concentrate on large-scale, commercial production of the powdered form of the alloys. The Colorado School of Mines will research ways to minimize the effect of corrosion on battery performance.

Turning metal into powder

In addition to assisting Ovonic Battery with the development of the alloy, Ames Lab has another crucial task. During the next two years, Pecharsky, Anderson and Foley will research the most efficient, cost-effective way of turning the alloys into versatile metal powder.

"There's no easy way to manufacture sheets or wires or screens out of these types of materials because the alloys are intermetallic compounds, and they are brittle," Pecharsky says. "The basic way hydrogen-storage alloys are used in batteries is in the form of powders.

Jim Foley (left) and Vitalij Pecharsky have high hopes that the HPGA process will produce high-quality, long-lasting alloy powders for rechargeable batteries.

"The Ames Laboratory is the leading laboratory in the metallurgy field."

A powder is much more flexible."

Turning the alloys into fine-grained metal powders is no easy task, though. Most commercial powder producers cast the molten alloy into ingots weighing several hundred pounds, let them solidify and then grind them into powder. But this process can take days, and because the metals within the ingot segregate during the solidification process, the resulting powder particles do not all have the same chemical composition. "It gives you inconsistent quality," Pecharsky says.

The Ames Lab team believes the best way to process the magnesium alloys will be through a technique known as high-pressure gas atomization (HPGA), which excels in producing ultrafine powder particles.

In HPGA, a stream of molten material is blasted with extremely cold argon or helium gas at up to three times the speed of sound. This converts the material into fine liquid particles that solidify quickly and are nearly spherical in shape. Because of the rapid solidification, the particles have virtually identical chemical compositions. Pecharsky says the homogeneity of the HPGA powder is a big advantage over the powder made from crushed ingots.

"With HPGA, essentially 100 percent of the yield is the target alloy," he says, noting that the resulting powder is also cleaner because it doesn't require any additional grinding.

Anderson says the HPGA – produced powders will also be more powerful and will enable the metal-hydride batteries to last longer. "A clear performance advantage we expect for the spherical atomized powder is a much longer cycle life in rechargeable batteries," he adds.

The new generation of rechargeable batteries won't contain lead and cadmium, which are environmentally harmful materials.

In fact, the metal-hydride batteries may well outlast the products they power. "When electric cars become more of the norm, the body of the car will need to be replaced before the batteries have reached their useful lifetime," Foley says.

Cutting costs

Using HPGA would make the processing simpler, faster and less expensive than current methods – a crucial step in lowering the overall price of metal-hydride batteries and fuel cells.

"Right now, a lead-acid car battery costs $40 to $50. If you wanted to replace it with a nickel metal-hydride battery, you would be looking at $300 to $400, and that would be a tough sell," Pecharsky says. "But if the cost of the battery could be reduced to around $100 per battery and it was smaller, much lighter, much safer and stored much more energy, people would start buying those batteries."

Foley adds, "The three main hurdles to getting metal-hydride batteries into the mainstream are cost, weight and performance. We think that our knowledge of materials and processing can overcome most, if not all, of those hurdles."◆

For more information:

Vitalij Pecharsky, (515) 294-8220
vitkp@ameslab.gov

Iver Anderson, (515) 294-4446
andersoni@ameslab.gov

Jim Foley, (515) 294-8252
foley@ameslab.gov

Current research funded by:

Department of Commerce, National Institute of Standard's Advanced Technology Program

DOE Basic Energy Sciences Office

On Thin Ice

by Susan Dieterle

Jim Liljegren believes data from the microwave radiometer will provide a better picture of the relationship between polar clouds and global warming.

The popping and exploding Jim Liljegren heard on July 4, 1998, didn't come from fireworks.

It came from arctic ice being crushed beneath the hull of an icebreaker that was carrying Liljegren toward the solid footing of the North American mainland for the first time in eight weeks – two weeks past his scheduled June 23 departure date.

The ice pack surrounding the ship where he had been stationed was cracking and melting, making it impossible for the scheduled plane to land safely. He was forced to wait until a second icebreaker, the *Polar Sea*, could pick him up along with the 13 scientists and 18 crewmen due to leave with him.

Extreme vigilance had been a necessary part of his life for the past two months. Before taking each step, he had carefully probed the ice in front of him to make sure he didn't sink into a slushy hole where the underlying ice was only a few inches thick. And he had warily watched for polar bears prowling the ice in search of seals – or anything else – to feed on.

Those two months had given him a firsthand view of both the harshness and the wonder of nature. As the *Polar Sea* bucked through the expansive ice pack, propelling itself on top of the ice until the sheer weight of the ship crushed through the 12- to 16-foot-thick floe, Liljegren thought about the ups and downs of his experience.

"It was hard not knowing when we would be able to leave," he says. "But it was wonderful to see all of the things you'd read about or modeled actually occurring. It was fantastic."

Liljegren, an atmospheric researcher at Ames Laboratory, was one of several scientists from throughout the world who volun-

The Canadian Coast Guard's *Des Groseilliers* sits in the heart of the drifting arctic ice pack.

Throughout his two-month stay, Liljegren and other scientists checked instruments in the outlying ice camps (pictured left) and kept an eye on data transmissions aboard the ship.

teered for a six-week shift aboard the *Des Groseilliers*, a Canadian ice-breaker intentionally frozen into the arctic ice pack for 13 months to study polar climate conditions. The *Des Groseilliers* mission is at the heart of a five-year climate study funded by the National Science Foundation and the Office of Naval Research. Data collected during the mission will be used to improve the accuracy of climate models in order to make better predictions of how global warming might affect Earth's climate.

Polar data is crucial; most of the sun's heat strikes Earth at the equator and is then carried toward the poles where it dissipates back into space. Unless the models contain accurate information on the interactions of water, air and ice at the poles, their predictions will be faulty. Prior to the *Des Groseilliers* mission, it had been more than 100 years since the last long-term study of the arctic climate.

Liljegren's involvement with climate research began seven years ago when DOE was looking for volunteers for its Atmospheric Radiation Measurement (ARM) program, which studies the role played by clouds in maintaining a balance between incoming heat from the sun and outgoing heat radiating from Earth. Liljegren, then a mechanical engineer at Pacific Northwest National Laboratory in eastern Washington, was intrigued.

He began working with ARM's microwave radiometers, sensitive radio receivers tuned to the frequencies at which water vapor and liquid water emit tiny amounts of energy. The strength of the signals indicates the amount of water vapor in the atmosphere and liquid water in clouds. Clouds play a critical role in climate models and in the ongoing debate over global warming. Liljegren notes that although carbon dioxide is the trigger for the so-called "greenhouse effect," water vapor is the controlling factor in the phenomenon.

"You get this sense of smallness because the ice seems to go on forever."

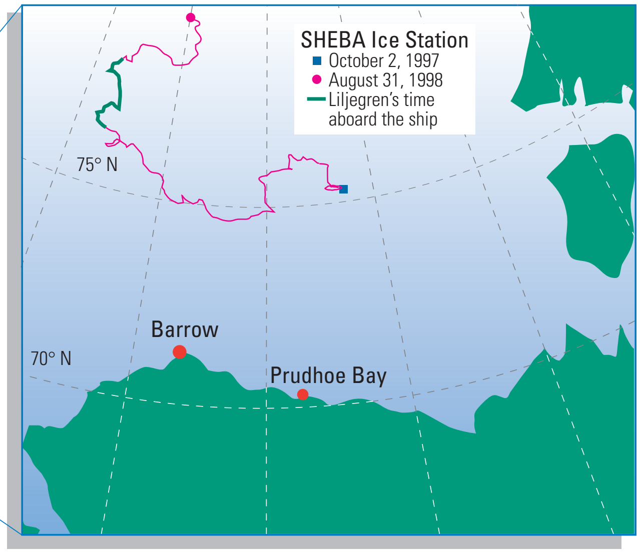
"Doubling the carbon dioxide concentrations produces only a slight warming in Earth's atmosphere, but because most of Earth is covered with water, this warming will cause more water to evaporate into the air," he says. "Water vapor blocks heat from escaping to space, so this causes additional warming, which causes additional evaporation, and so on.

"But sooner or later, water vapor condenses into clouds, which are made of liquid-water droplets or ice crystals or both. Liquid-water clouds are very effective at keeping heat from escaping Earth's surface, but they also tend to cool the planet."

For now, scientists don't know whether an increased cloud cover would enable Earth's climate to balance itself or cause atmospheric temperatures to escalate. To gather the needed cloud data from a variety of longitudes, ARM has radiometers at three strategic sites: the Great Plains in Kansas and Oklahoma; in the equatorial region near New Guinea; and at Barrow, Alaska.

When the National Science Foundation began planning an in-depth study of the arctic climate, they wanted ARM to participate. The study is known as the Surface Heat Budget of the Arctic Ocean, or SHEBA. As part of the overall five-year SHEBA project, one year would be spent on the ice pack gathering polar climate data, and the next four years would be spent analyzing the data and applying the findings to climate models.

Among the instruments ARM



sent to the SHEBA site was a microwave radiometer, which made Liljegren eligible for a six-week shift. Even though cold temperatures aren't his favorite ("I put on a sweater when the air conditioner is on," he says with a laugh), he eagerly signed on.

He wanted a shift in the early summer when the sun is up continuously so he could see the clouds the radiometer was measuring. Fortunately for him, that also meant relatively warmer temperatures and a better chance of spotting polar bears that might be lurking near the ship. He and the other scientists received gun-safety training in case of a polar bear attack.

On May 11, he traveled to Barrow, located on the northernmost tip of Alaska. From there, he boarded a Twin Otter plane along with a fresh rotation of scientists and crewmen and a load of supplies. The plane flew to the SHEBA site every three weeks for personnel exchanges and supply drops and was the sole source of transportation between the ice camp and the mainland.

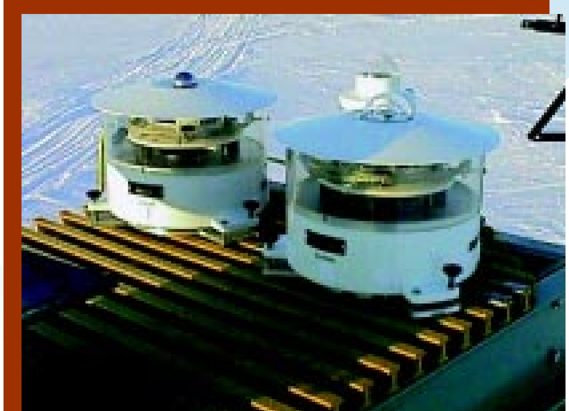
During the two-hour plane flight, Liljegren was struck by the vastness of the ice pack. "You get this sense of smallness because the ice seems to go on forever," he says. "You realize how very hostile the environment is."

Life in the Arctic took some getting used to. Because the sun never set and because there was so much to learn at first, Liljegren sometimes found himself staying up for 20-22 hours straight. He gradually developed a routine so that he'd know when to sleep. Each day, he would check the data recorded during the night by the various ARM instruments, and then physically inspect each instrument to clear moisture from the lenses, re-level the stands that shifted in the melting ice and make sure they were positioned properly to track the sun. He also helped other SHEBA scientists, sometimes standing guard for polar bears while the researchers checked their instruments on the ice.

Venturing onto the ice was never an easy task. Though temperatures seldom rose above freezing, the wind chill made it as cold as 40 degrees below zero. "You couldn't just take a little walk around the ship," Liljegren recalls. "First, you had to dress appropriately, then you had to check out a radio and a gun and you had to let the bridge know where you were going and stay in contact with them. At first it seemed a little burdensome, but you had to take reasonable precautions to be safe."

Fog and snow frequently shrouded the ice pack, making it difficult for scientists to see the ship from the instrument sites – and making it difficult to spot an approaching polar bear. There were no

In addition to the microwave radiometer, Liljegren was responsible for checking other ARM solar and infrared radiometers.



Fog and snow frequently shrouded the ice pack, making it difficult for scientists to see the ship from the instrument sites – and making it difficult to spot an approaching polar bear.

Melt ponds (left) were common on the ice; (above) the U.S. Coast Guard's *Polar Sea* carved its way through the ice to pick up Liljegren and the others.

polar bear attacks, although seven bears were sighted during a two-week period beginning in late May.

Anytime a bear got within 1,000 meters of the ship, crewmen set out on either snowmobiles or the helicopter to chase it away. With the scientific staff spending several hours each day out on the ice, a hungry bear would have posed a real threat. By keeping the bears clear of the SHEBA site, neither the bears nor the group members were harmed.

A different kind of danger gurgled beneath their feet. The ice pack melted more rapidly than expected. Large cracks, known as leads, fractured the ice floe. Near the end of May, the crew tied the ship to large mooring posts that had been driven into the outlying ice, a precaution designed to secure the ship and keep the ice from shifting as it started to break up. By mid-June, the ice immediately around the *Des Groseilliers'* hull had melted, allowing the ship to float within the ice pack.

Melt ponds now covered the ice. Ponds with white bottoms indicated that somewhere below the slush was "multi-year ice" that would never completely melt and would support Liljegren's weight as he stepped on it. Darkened melt ponds, however, indicated that the ice was only a few inches thick.

Life inside the ship was less forbidding. His 8' x 12' cabin was comfortable, and the food was exquisite. The chefs aboard the *Des Groseilliers* whipped up lavish Sunday brunches and hearty meals. The food served its purpose. The grueling work in frigid temperatures was physically exhausting, so the researchers and crew needed to eat well to keep up their energy levels.

The group also made time for fun. Liljegren visited with his counterparts during the ship's bar nights and attended a few theme parties, including a beach party where he showed off a Hawaiian shirt he'd brought along. "Everybody that I worked with was really nice – not just professionally, but personally," he says. "All of the people involved were committed to making it a good experience."

At the weekly SHEBA science meetings, Liljegren listened as his fellow scientists explained their work and how the various elements of the arctic ecosystem worked together. He gained a greater appreciation for the way vegetation and animals adapt to the forbidding environment. "The Arctic is prolific in terms of life, although you don't always notice it," he says.

He also managed to find a few moments of solitude. "Every now and then in the evenings, I would go out and just stand on the bow of the ship and look out because it was so unique to see the sun shining at midnight, reflecting off of the melt ponds. It was amazing, really."

Liljegren says he was pleased with the radiometer's performance at SHEBA and is looking forward to analyzing all of the data. "It looks like it's going to give us a really useful picture of the role of polar clouds and of the radiation transfer through the atmosphere," he says. "Everything worked quite well, so we certainly have the data to move forward."

But even as he moves ahead with his work, he looks back with satisfaction at his time in the Arctic. "It was a very unique experience being in a place where almost no one else has been," Liljegren says. "Working and living there for two months was fantastic."◆

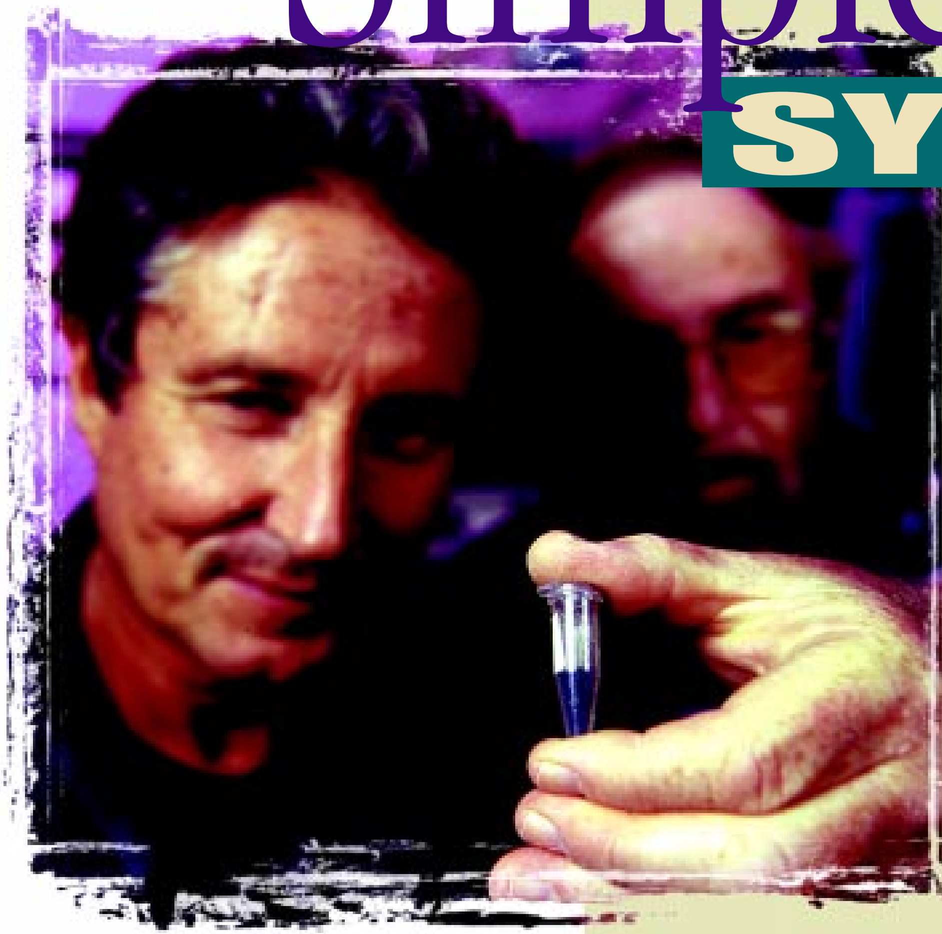
For more information:

Jim Liljegren, (515) 294-8428
liljegren@ameslab.gov

Current research funded by:
DOE Biological & Environmental Research Office

Simple SYSTEMS

by Saren Johnston



The experimentalist, Ferdinando Borsa (foreground), and the theorist, Marshall Luban, examine a sample of manganese 12, a material with potential applications in the computer industry.

Researchers are exploring the enticing world of molecular magnetic clusters

In the furthest stretches of their imaginations, physicists never believed they would have molecular structures in which they could embed small geometrical arrangements of interacting magnetic ions. But now that chemists have become remarkably adept at preparing such structures, physicists have access to the kinds of uncomplicated systems they need for investigating magnetism at the fundamental level.

And, although they may be a long time coming, the potential applications for molecular magnetic clusters, especially in the field of computing technology, are staggering. Each molecule can be viewed, in certain cases, as a microscopic magnet with magnetization that can be oriented up or down, thus carrying a bit of binary information.

Imagine data-storage capacities thousands of times greater than what are available in today's computer systems. Magnetic molecular clusters may one day make it possible to stockpile hundreds of gigabytes of data in an area equivalent to the head of a pin, an astounding feat when you consider that just 1 gigabyte can store enough information to fill 62,500 typed, double-spaced pages.

Beyond the incredible data storage possibilities, there also exists the prospect that these clusters could be manipulated at the atomic level to form logic components in a quantum computer. Quantum computers would operate at speeds hundreds or thousands of times as fast as the supercomputers that amaze us today.

Another fascinating, potential spinoff of the study of magnetic clusters is the connection with magnetic molecules that are present in biological systems and whose functions are still largely unknown. But before we look too longingly at what might eventually develop from the study of molecular magnetic clusters, a great deal of fundamental research must still be done.

In the molecules of interest, there are as few as 12, 10, six or even four atoms grouped together, with each atom having a net magnetic moment. Because these magnetic moments arise from the intrinsic angular momentum, or spin, of the atomic electrons, physicists frequently refer to the magnetic interactions among "spins."

Driven by an enthusiastic curiosity about these systems, Ferdinando Borsa, an Ames Laboratory senior physicist, is carrying out nuclear magnetic resonance (NMR) experiments with certain molecules to better understand their basic magnetic properties. NMR uses the spectroscopic properties of the energy levels of the magnetic and quadrapole moments of the nuclei in strong magnetic fields to obtain microscopic information about the atomic magnetic moments, or spins, in the molecules. This information may ultimately provide scientists greater knowledge about the magnetic properties of more complex materials and make it possible to design materials with specific characteristics.

"Teach us Delight in simple things."

Puck of Pook's Hill, The Children's Song
- Rudyard Kipling

The structures Borsa is investigating are unique because, although the small molecular structures chemists have designed contain many different atoms, the magnetic properties of those molecules are determined by only a handful of interacting magnetic ions arranged in very ordered ways.

"The beautiful thing about these molecules is that for the first time it's possible to control the number of magnetic moments," says Borsa. "You can also control where they are located in the molecule, their distance apart and what kind of interactions take place among these moments. So these very simple systems are ideal model systems for doing theoretical calculations that are almost exact and can be compared directly to the experimental data." Developing analytical theories based on these model systems should allow scientists to accurately predict the magnetic properties of the molecules as a function of parameters such as temperature and applied magnetic field.

Marshall Luban, also an Ames Laboratory senior physicist and a collaborator with Borsa on the research, is involved in the theoretical aspects of small magnetic systems. He joyfully notes that the structures chemists have created in the laboratory are a theorist's dream. "They're a kind of utopia – simple systems with just a few interacting ions as opposed to a number such as 10^{23} power, which you might normally worry about," he says. "Those kinds of problems are so difficult that it's a pleasure to be able to work on something far simpler, the other end of the spectrum in range of difficulty. What we're talking about, in a sense, are realizable toy systems that are ideal for theoretical calculations."

Borsa adds, "In more complicated systems, there is a big gap between the theories and the experiments. The experiments allow you to get some information on magnetic properties, but when you want to reproduce that with a theory, you have to use approximate theories or use computer simulations on a small number of particles and extrapolate the large numbers. With these small systems, you don't need to do all that because you only have six, 10, 20 spins – you can solve the problem exactly."

Zeehoon Jang, an Ames Lab graduate student, is doing experimental work on small molecules with Borsa, but is also intrigued by the theoretical possibilities that are Luban's specialty. He has done many NMR measurements on small molecules and worked on some of the theoretical calculations associated with those molecules. "Zeehoon is our line of connection between the experiments and the theory," says Borsa.

Zeehoon Jang is ready to place a sample of manganese 12 in the Bath Cryostat, which will cool the specimen to below 4.2 Kelvin, the temperature of liquid helium, for NMR analysis. To achieve temperatures below 4.2 K, Jang will lower the pressure of the liquid helium in the cryostat.

"Order and simplification are the first steps toward the mastery of a subject ... "

The Magic Mountain
- Thomas Mann

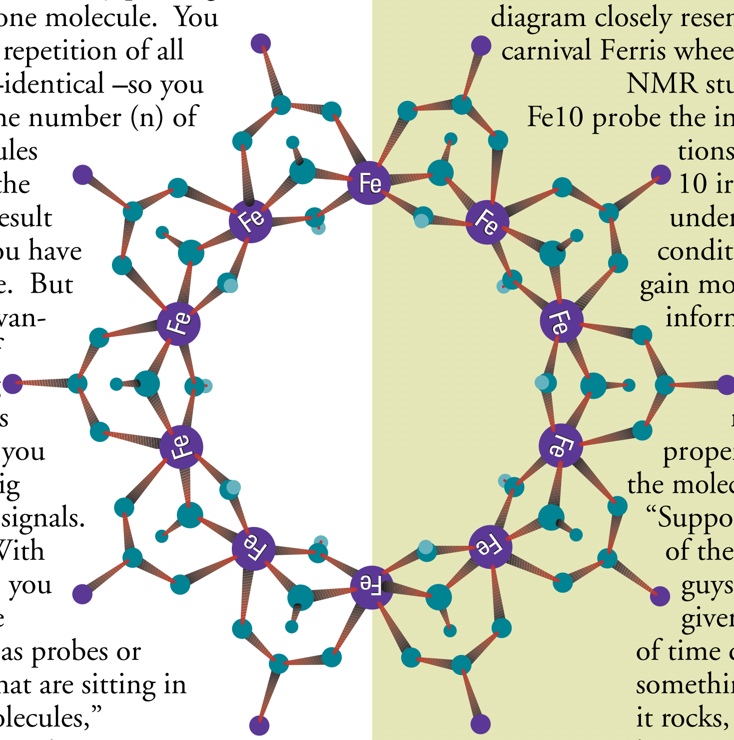
"I think physics is beautiful when it can be made simple," says Borsa. "The logical and mathematical tools are complicated, but you are aiming at simplicity in physics to get to the root of the problem."

The simplicity Borsa requires to get to the source of magnetic molecule puzzles is supplied primarily by Dante Gatteschi, a professor of chemistry at the University of Florence in Italy. Gatteschi and members of his research group, among them the brilliant, young researcher Alessandro Lascialfari, produce and characterize the new materials that provide Borsa the molecular systems he requires for his NMR investigations.

Although simple in terms of the number of interacting magnetic ions, these molecules are at the same time complicated, containing lots of organic materials, such as oxygen, carbon and hydrogen, which shield the magnetic moments from outside interference. "These materials serve as scaffolding," says Luban. "They keep the ions carrying the magnetic moments positioned as they are. If you ripped off this stuff, the ions would just wander away."

Borsa elaborates, comparing a molecule to a big ball. "The magnetic moments are inside the ball; they don't see each other, so the molecules act independently of one another. Although you have a number of these molecules in a crystal, when you do an experiment, you're essentially probing the behavior of one molecule. You have a repetition of all units –identical –so you have the number (n) of molecules times the same result that you have for one. But the advantage of having n times is that you have big NMR signals.

"With NMR, you use the nuclei as probes or spies that are sitting in the molecules," Borsa continues. "And what the nuclei see is the fluctuation of the spins. So you are studying the motion of the spins by looking at the effect on the NMR."



Fe10, the "ferric wheel," is one of the simple systems that may help physicists discover more about the collective behavior of particles.

"Our life is frittered away by detail. ... Simplify, simplify."

Walden. II, Where I Lived, and What I Lived For

- Henry David Thoreau

Some of the molecules that Borsa, Luban and Jang are investigating include: manganese 12 (Mn12), iron 6 (Fe6), iron 10 (Fe10), copper 8 (Cu8), copper 6 (Cu6) and, the latest addition, chromium 4 (Cr4). That translates to molecules with 12 or fewer spins, and Luban reminds us, "That makes for an enormous simplification in any effort or attempt to describe the magnetic properties of those molecules."

As an example, he invites us to look at a diagram of an Fe10 molecule, sometimes called the "ferric wheel," because ferric means made of, containing or derived from iron; and because the Fe10 structure diagram closely resembles a carnival Ferris wheel.

NMR studies of Fe10 probe the interactions of the 10 iron ions under various conditions to gain more information on the magnetic properties of the molecule. "Suppose one of the iron guys at a given instant of time does something, say it rocks, rotates in space or jumps – it screams," says Luban, anthropomorphizing the iron ions. "Then we ask the question: 'If this guy screams now, at this place, what impact does it have elsewhere at these other iron locations at a later time?' This is called the equilibrium/time correlation function."

Because of the simplicity of the Fe10 system, there's a good chance that Luban may be able to calculate the equilibrium time correlation function from first principles (i.e., without approximations or modeling). He can then directly compare his predictions about the magnetic properties of Fe10 with Borsa's experimental data. "Hopefully, they will be in pretty good agreement," Luban says. "Then we will be able to say, 'Yes, we can in fact predict all of the properties of this system.' The applications, I think, will be forthcoming. The more we understand from these simple systems, the more we can predict. Then we can start to get greedy and design systems that will exhibit the properties we would like."

Borsa and Jang hope the NMR measurements they do on these various systems will give them a better idea of how the fundamental physical law for magnetism determines the magnetic behavior of interacting spins. "If we can understand that, we may be able to design a material that will work for better computer magnetic memory," says Jang.

Borsa admits that application is down the road. Right now, he's happy to indulge his curiosity by using these simple systems to observe how particles behave when they are coupled together. "One of the fundamental problems in condensed matter physics is what makes many particles behave in a collective way," says Borsa. "Why would a bunch of particles, when they're together, have some new behavior that is not a direct consequence of the addition of the behavior of each individual particle? The hope is to find some basic law that determines the collective behavior of particles, and then you can use it in any kind of field."◆

For more information:

Ferdinando Borsa, (515) 294-9901
borsa@ameslab.gov

Current research funded by:

DOE Basic Energy Sciences Office

The Dragonslay

by
Susan Dieterle

Researchers Matt Kramer (left) and Mufit Akinc

Think back to the lore of Hercules' battle with the Hydra and you'll understand science's frustrating search for a material that can withstand high temperatures.

The Hydra, a nine-headed serpent that Hercules was bidden to slay, was a formidable foe: every time Hercules cut off one of its heads, two more would grow to replace it. Even for a man possessing the incredible strength of Hercules, it was an exhausting task.

The mythical battle has modern-day parallels. Scientists are searching for a new material that can withstand temperatures of up to 1600 C (2900 F). It would replace steel and other alloys in jet engines, car motors, furnaces and turbines, and would allow fuel to burn hotter and more efficiently. However, they haven't found a material that possesses all of the necessary attributes. Every time they try a new material, new "heads" pop up:

- if the material can withstand high temperatures – pop – it rusts in the presence of oxygen,
- if it doesn't rust – pop – it sags at high temperatures, and
- if it doesn't sag or rust – pop – it melts as the temperatures climb.

But the battle is far from over. Scientists across the country have united behind a material whose promising properties were discovered at Ames Laboratory. By surrounding the problem with a multi-lab effort, they hope to lop off the remaining heads and slay the dragon once and for all.

"That's how research is," says Mufit Akinc, an Ames Lab senior ceramic engineer and chair of the Materials Science and Engineering Department at Iowa State University. "You go one step at a time."

Akinc is working with molybdenum-silicon-boron (Mo_5Si_3B), the material at the center of a five-year project funded by the DOE. Participating scientists from nine labs, including Ames Laboratory, are trying to work out the kinks in the intermetallic compound and make it viable as the high-temperature material of the future.

Akinc took up his sword in the battle six years ago when Pat Thiel, director of the Lab's Materials Chemistry Program, suggested that he take a fresh look at silicides as a high-temperature material. Silicides are compounds made of silicon and other elements. They have high melting points, but some silicides are prone to oxidation, a corrosion process that causes them to degrade in the presence of air. Other silicides have poor creep strength, meaning that they deform or sag at high temperatures.

Several decades ago researchers discovered molybdenum disilicide ($MoSi_2$), which withstands temperatures of more than 1600 C without oxidizing, but sags in the intense heat. "It has no strength at that temperature," Akinc says. The material is used as a heating element in furnaces, since strength isn't needed in that kind of an application.

To work in the next generation of jet engines and other load-bearing applications, researchers want a material with oxidative stability and good creep strength at temperatures of at least 1400 C (2000 F). "It may sound very simple, but it's so drastic," Akinc says. "You're getting into a temperature regime where the material becomes almost white-hot. So far, no one has been able to get a material that, at this kind of temperature, won't melt, sag or deform, or oxidize in the presence of air."

Akinc began working with a Mo_5Si_3 alloy, which had strength but poor oxidative stability, and employed a "doping" technique used by Ames Lab senior chemist John Corbett. Doping involves introducing small amounts of a new element in order to dramatically change the properties of the original material. Akinc discovered that when Mo_5Si_3 is doped with boron, the oxidation problem is virtually eliminated. "This material essentially meets all of the molybdenum disilicide ($MoSi_2$) performance with respect to being able to stay at 1600 C and being able to resist oxidation, but it's at least 10 to 100 times more resistant to deformation," he says.

As he continued investigating Mo_5Si_3B with the help of former graduate students Mitch Meyer and Andy Thom, word about his work began to spread. One of the students approached Matt Kramer, assistant program director for Metallurgy and Ceramics, for help in understanding the deformation processes affecting the alloy. Kramer was intrigued by the material's properties and began doing some microstructural characterization work.

The material's properties also caught the attention of associate metallurgist Bruce Cook and associate ceramist Ozer Unal. Cook is measuring the electrical properties of the material, while Unal is concentrating on its mechanical properties.

Scientists throughout the nation also were interested. Last year the Ames Lab group received a three-year, $900,000 grant from DOE's Advanced Energy Projects Division to continue work on the molybdenum-silicon-boron material.

In 1996, DOE wanted to select a high-temperature intermetallic substance for a five-year, multi-lab study. "They wanted something that would leapfrog the current technology, not something that just moved it ahead in small increments," says Kramer, who presented the proposal from Ames Lab suggesting Mo_5Si_3B for the project.

Other materials that were discussed included iron-aluminides and nickel-aluminides. "Most of the iron- and nickel-aluminides had a maximum operating temperature of 800 C to 1000 C," Kramer says. "We had already pushed the molybdenum material to almost 1400 C, so this fit very well with what the DOE was looking for."

To avoid contamination, pellets of the silicide material are studied in the oxygen-free atmosphere of a glove box.

The molybdenum-silicon-boron material was selected for the Design and Synthesis of Ultrahigh Temperature Intermetallics Project. DOE is dividing $300,000 a year among the eight participating national labs – Ames Lab, Argonne, INEEL, Lawrence Berkeley, Lawrence Livermore, Los Alamos, Oak Ridge and Sandia – and the University of Illinois. The funding is helping to redirect research efforts toward Akinc's material and to stimulate collaborative efforts among the 25 scientists involved in the project.

The two project coordinators are R. Bruce Thompson, director of Ames Lab's Nondestructive Evaluation Program, and Roddie Judkins, manager of the Fossil Energy Program at Oak Ridge.

Thompson, who also directs Iowa State's Center for Nondestructive Evaluation, says that even though the project is in its early stages, it is already generating a lot of excitement in several scientific disciplines. "There's a tremendous amount of interest in this material and the questions it opens up, both scientifically and technically. Given the creative talents of the scientists involved, that should lead to something quite useful," he says.

Judkins notes that use of the molybdenum material could help the environment. If the operating efficiency of turbines and engines improves, less fuel would be needed to generate the same amount of power. Using less fuel would also cut the amount of emissions and "greenhouse gases" in the atmosphere, thereby reducing the threat of global warming.

"...the public good derived from this is energy security and an improved environment."

"I think this project clearly falls under the category of public-good R&D, and the public good derived from this is energy security and an improved environment," Judkins says.

Even though the molybdenum-silicon compound represents a large step forward in the search for a new high-temperature material, several problems remain.

Mo_5Si_3B, like many other high-temperature intermetallic compounds, is extremely brittle at room temperature. "It's not a very tough material," Akinc says. "You can hammer steel and it won't do any damage, but if you put this material at an angle and whack at it, you can break it. You don't want that to happen to an airplane engine."

It's also difficult to process. "Processing means you have to synthesize the materials and turn them into certain shapes. This material is extremely difficult to deform at high temperatures and has great strength," Akinc says. "That's good, but not if you're trying to shape it."

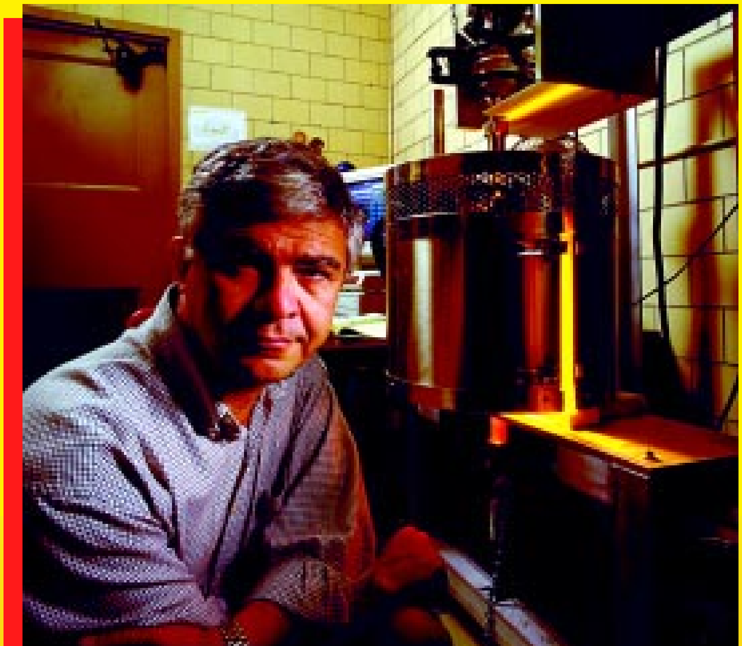
That's not all. "In order to cast the material from the molten state, you need to heat it to 2200 C," he says. "How do you melt it and where do you melt it? And how do you pour it into a mold that will withstand that kind of temperature? These are the problems we need to work out."

The DOE labs are tackling different aspects of those problems, and the researchers hope their combined efforts will make the material viable. "We're making significant progress in a relatively short amount of time," Judkins says. "We have some of the best people at some of the best labs doing the work on this. We've got a lot of good science in this investigation. That's one reason I think it will be successful."

Aside from the work on the material itself, Kramer says the multi-lab effort represents an enormous achievement. "One of the objectives of the project is to get the labs to work together, and regardless of whether the project works or doesn't work in terms of the technology, it really has helped the collaborative research," he says.

Akinc believes this kind of unified effort is the best hope for slaying the high-temperature beast. "It takes perhaps one person to see an opportunity, but it takes a large team of scientists with different backgrounds to turn it into a reality," he says. "That's what we're doing."

With that upbeat attitude, "heads" are sure to roll.◆



Akinc tests the mettle of the intermetallic compound in furnaces that reach temperatures of 1700 C.

For more information:

Mufit Akinc, (515) 294-0744
makinc@ameslab.gov

Matt Kramer, (515) 294-0981
mjkramer@ameslab.gov

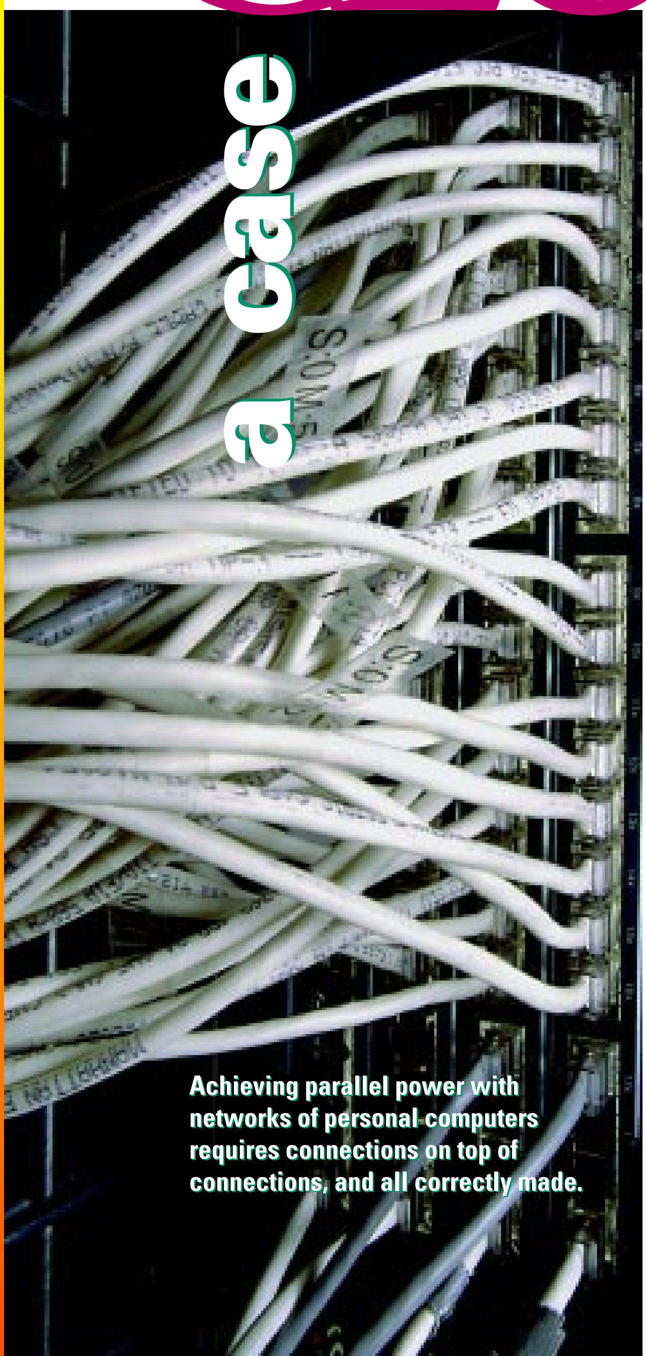
Current research funded by:
DOE Basic Energy Sciences Office

a case for CLUSTERS

Supercomputing by Way of Personal Computer Networks

by Saren Johnston

David Halstead (standing) and Mark Gordon are working to improve the communications among personal computers in network clusters. Their efforts are helping to make parallel computing power available for greatly reduced costs.



Achieving parallel power with networks of personal computers requires connections on top of connections, and all correctly made.

Until very recently, parallel computing came in a box – an incredibly expensive one. Inside a boxed system is an activity center comprised of anywhere from several to many thousand central processing units (CPUs) that interpret data and execute instructions. It's like packing the processing power of a whole warehouse of computers into a shipping crate. What you get is a supercomputer, but that much power comes at an outrageous price.

Just one such boxed system can cost millions of dollars, and what if one or two CPUs go bad? How do you fix a supercomputer? Mark Gordon, Ames Lab program director for Applied Mathematics and Computational Sciences, explains the reality of supercomputer repair. "You pay the manufacturer 10 to 20 percent of the purchase price each year for maintenance," he says. "You can't get them fixed anywhere else."

Out of the box

But high-performance parallel computing doesn't have to cost a fortune. Gordon and several of his colleagues at Ames Laboratory's Scalable Computing Lab (SCL) are determined to make traditionally expensive supercomputing capabilities more economical and attainable for scientific and educational communities.

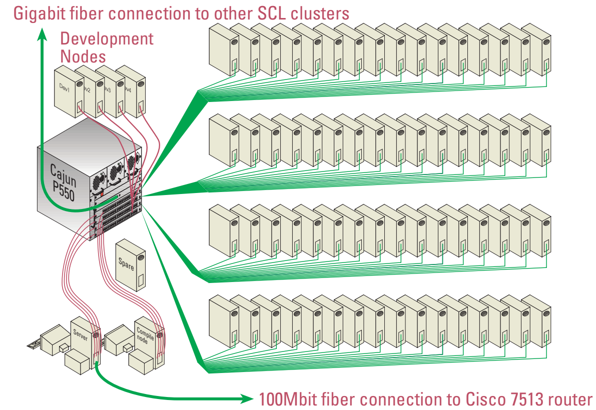
Playing an intriguing game of "workstation upset," Gordon and SCL researchers David Halstead, John Gustafson, Stephen Elbert, Don Heller, Dave Turner, and Bruce Harmon are dumping the traditional concept of boxed-system supercomputers. Incorporating the option to grow, or scale up, they are taking computing power out of the box and spreading it over networks of personal computers (PCs), creating clusters that operate at speeds comparable to today's best parallel computers, and for a fraction of the cost.

Parallel computers are like valued employees: they can handle a number of tasks at the same time. Their multiple processors work simultaneously on different parts of a single problem, making them far more efficient and able to handle more complex problems than sequential computers, which tackle problems one step at a time.

One of the ways the SCL team

hopes to make parallel computing more economical is by devising a “cluster cookbook” for the world wide web, which will provide guidelines on how to construct PC clusters. Team members also plan to develop and host a hands-on workshop that will help bring the cost-saving cluster computing technique into university departments, individual research groups and the classroom.

How many shelves does it take to hold the 64-node ALICE cluster? Four in a tidy diagram, but a few more in the lab.



64 node/128 processor Ames Lab/ISU Cluster Environment

Each personal computer in the SCL’s 64-node cluster contains two central processing units, making a powerful system of 128 processors.

The cluster craze

“What precipitated the clustering effort is that in the last few years manufacturers of personal computers have been making them with speeds that are equivalent to workstations,” says Gordon. “This means that you can take these computers as individual units and use them for really high-performance computing in a sequential sense. You can put on one $3,000 personal computer what you used to put on a high-performance workstation, and it will perform just as well for you.

“What’s hard is going the next step: networking clusters of these PCs to make a true, parallel, high-performance computer that’s competitive with boxed systems that cost millions of dollars,” Gordon says.

Gordon and his colleagues have made that intricate job look easy. “It’s clear that small clusters work, small being eight,” he says. “We have a math cluster with eight nodes running partial differential equations. And all of our quantum chemistry codes can run in parallel.” Gordon adds that in other areas of the Lab, clusters of eight PCs are doing materials simulations and modeling new materials with desirable magnetic properties. “So the issue is, does clustering work when you scale up to 64? Does it work when you scale up to 128? That’s really unknown.”

Reality check

Whether larger networks of PC clusters will work depends to a great extent on how well researchers can optimize message-passing between the various computers in a cluster. The communications system currently in use is called gigabit, which is supposed to be several times faster than previous systems. But the performance has not matched the prediction. So part of the SCL team’s research is to determine how best to optimize gigabit.

“The Achilles’ heel of PC clusters in the past has been the communications capabilities,” says Thom Dunning, Battelle Fellow in Computational Sciences at Pacific Northwest National Laboratory. “And that’s one of the major problems they’re looking at here at Ames Lab. So they’re tackling what is probably the most significant problem in realizing the potential that PC clusters have.”

Configuration also has a lot to do with how well large networks of PC clusters perform. “Imagine having 64 PCs,” says Gordon. “You can arrange them in lots of different ways, and the further one computer has to go to communicate with another, the more arrangements you have. So there’s a traffic-directing problem to deal with.”

In addition, Halstead reminds us

“Cluster computing is a happy synchronization of technologies.”

of the obvious issue. "There's a definite storage concern for a large cluster network. Where do you put the thing? Also, all the energy that goes into a computer comes out as heat, so you'll use more power for air conditioning."

Cluster luster

SCL researchers believe the potential benefits of scalable cluster computing far outshine the issues they are working to resolve. A big advantage of taking the cluster path to parallel computing is that you can always reconfigure the system to meet the needs of the day. For instance, instead of having a 128-node computer, you might choose to have two 64-node computers. "You can set these things up as a computer lab, launch them to run a word processing program for a class, and reboot them to run as a single parallel computer," says Halstead. "You can trade off with other departments – whatever you want to do. With this kind of sharing of resources, you're only really limited by curriculum originality."

Halstead also notes that although PC clusters are not meant to replace the powerful supercomputers that operate at Department of Energy national labs, they can lessen the computing burden placed upon these machines and so reduce the barrier to national computer use.

Dunning explains, "The bigger systems are very full – they're oversubscribed because far too often we go to the big machines to solve routine problems. We're not taking advantage of the economics that could come if we had tiers of computing capability designed for specific tasks. I see PC clusters as being very effective at satisfying an intermediate set of demands that would then free up the big supercomputers to do the job that they are really intended to do, which is the very high-end computing."

Without a doubt, however, the biggest advantage of PC clusters is their low cost.

"Cluster computing is a happy synchronization of technologies," says Halstead. "If a PC dies, you throw it away and go down and buy another one, kind of like replacing a fan belt. The beauty is if a particular PC is not needed in a cluster, it's still a very powerful desktop machine. We're not buying into a hardware technology that in a year's time will be completely useless due to lack of software support."

Maybe the answer to whether clusters will work when scaled up to larger and larger systems will come soon. The SCL team recently constructed a cluster of 64 PCs, each with two central processing units, and is now testing its ability to perform parallel computations.

Halstead has high praise for the ISU students employed by the SCL, noting that the cluster, fondly named ALICE (Ames Lab/ISU Cluster Environment), was made possible by their extensive knowledge of the operating system and network communication protocols. The students include Vasily Lewis, Brian Smith, Chris Csanady, Stephanie Holeman and Chris Williams. "Vasily was responsible for the design and implementation of the ALICE compute node, the ease of which is essential to the project," Halstead says. "And Brian produced a cluster monitoring tool that allows the status of the cluster to be ascertained using a web browser. The talents of the entire student group were invaluable in addressing the difficult issue of configuring 64 PCs so that they act as a single computer.

"At the end of the day, this thing should be four times as fast and have four times the storage capacity and memory as the largest supercomputer in the SCL, which cost just shy of a million dollars," says Halstead. "So it's four times as fast for a third of the price."

"So it's four times as fast for a third of the price."

The SCL researchers have compared the performance of their clusters with that of commercial parallel computers by using a computer benchmark called HINT, which Gustafson developed and for which he earned an R&D 100 Award in 1995. "I think HINT is better than just about any other way of benchmarking computers," says Gordon. "If you take John Gustafson's method and evaluate our clusters against one of the best parallel computers on the market today and then go the next step and divide that by the cost to get the price/performance ratio, the clusters blow everything else away. And that's our point – not to show people how to do really great parallel computing because lots of people can do that, but to show them how they can do it in a very cost-effective way."◆

For more information:
Mark Gordon, (515) 294-0452
gordon@ameslab.gov

David Halstead, (515) 294-1943
halstead@ameslab.gov

Current research funded by:
DOE Basic Energy Sciences Office

Seeing the Forest from the Trees

by Steve Karsjen

On this day there are six large white boxes stacked neatly along the wall of Roger Jones' laboratory. The boxes each contain several bags of wood chips from Douglas Fir trees. Each of the chips ranges in size from approximately an inch to an inch and a half long to about an inch wide. Altogether there are thousands, perhaps hundreds of thousands of wood chips in the boxes, which have been shipped to Jones by the Weyerhaeuser Paper Company, an industry giant in the making of paper and paper products.

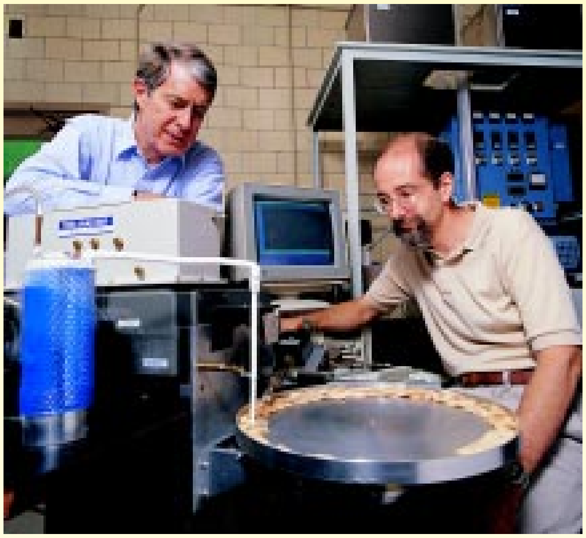
Weyerhaeuser has supplied the wood chips as part of a three-year research project in which Ames Laboratory scientists are participating to improve paper-industry techniques for analyzing the major components of timber harvested from forests across America.

The Ames Lab research revolves around the use of Transient Infrared Spectroscopy, or TIRS, which was invented by Jones, an Ames Laboratory associate chemist, and Ames Lab physicist John McClelland. TIRS relies on spectroscopy, the art of analyzing substances by measuring the radiant (light or heat) energy their molecules either emit or absorb and then interpreting the resulting electromagnetic spectra.

Wood chips of various shapes and sizes are being analyzed by TIRS for the paper industry.

The On-Line, Real-Time Advantage

Today manufacturers are most interested in the mid-infrared (mid-IR) portion of the spectrum (400 to 4000 cm-1), which contains an abundance of information about a material's molecular and chemical makeup. But solids, like wood chips, aren't popular in the mid-IR because they are thick and absorb infrared radiation. So in order to perform spectroscopic analysis of wood chips or other materials in the mid-IR region, technicians are forced to remove samples of the materials randomly from the process line, prepare thin or diluted specimens from the samples and then conduct the spectroscopic analysis in the laboratory. Thin samples are necessary to obtain useful spectra for analysis. If it sounds like a labor intensive, lengthy, and costly process – one that slows down the type of quality control necessary in the paper-making process – it is. "Of course, anytime you have to go off-line and into the laboratory, the measurement process becomes much slower and more expensive," Jones says.



John McClelland (left) and Roger Jones say the TIRS technology provides more detailed information than other analysis techniques being considered for use by the paper industry.

Whereas current technology is slow and cumbersome, the TIRS technique is fast and efficient, providing on-line analysis. TIRS actually takes advantage of the fact that the material, whatever it is, is moving down the process line. "The material has to be moving in order for TIRS to work," says McClelland.

TIRS can't actually make a thick material thin, but it can trick the infrared spectrometer into thinking that's the case. To do so, Jones reduces absorption by inducing a temperature transient in the moving surface of the wood chips as they move by on their way to the digestor that feeds into the paper machine. Gas jets blowing on the material temporarily create a very thin hot or cold layer at the surface of the material without physically thinning it. The mid-IR spectrum of the thin layer can then be measured by an infrared spectrometer.

Around and Around It Goes

With a laboratory model of a wood chip process line, Jones demonstrates the TIRS technique by placing wood chips on a large circular plate, which looks a lot like an oversized pizza pan. The chips are piled up along the outer edge of the plate and rotate with it as the plate spins around and around. At one point in the rotation, the chips come in contact with a hot blast of air from a gas jet, which strikes the surface of the chips, heating them. As the wood chips rotate through the field of view of an infrared spectrometer, the spectrometer measures the electromagnetic spectra of the heated sample. In Jones' experiment, the spectra being measured come from one of the major components of wood, lignin, the material that turns paper brittle and yellow over time. Low quality paper, like newsprint, contains a lot of lignin while most of the lignin is removed from high-quality paper. "By keeping track of how much lignin the wood contains, technicians control the quality of the paper they're producing," says Jones.

In addition to its on-line capabilities, TIRS conducts its analysis in real-time. "This is actually the most important aspect of TIRS," says McClelland. "Real-time measurement allows you to get data immediately so you can make adjustments that improve the quality of the paper on-line."

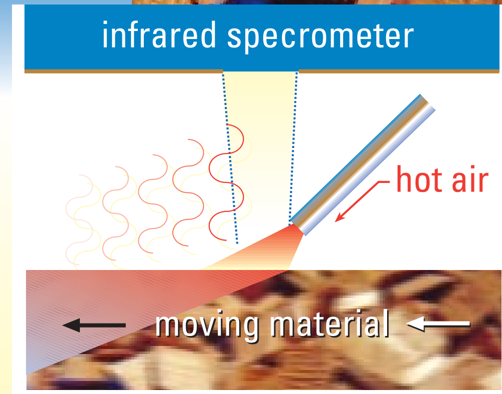
A Few Bumps Along the Way

Jones had a pretty good idea TIRS would provide the type of analysis the paper industry needs. Since its invention, the TIRS technology has been successfully used to analyze over a hundred materials from plastics to coal and corn. All of these samples were smooth, however, which is a far cry from the rough, irregular-shaped wood chip samples provided by the paper industry. There was also a question of whether the TIRS technology would work across tree species (hardwoods and softwoods) and on trees from all regions of the country. "Our model contains over a dozen species at this time," says Jones. "So far they haven't thrown anything at us that we haven't been able to analyze."

Where Do We Go From Here?

Although Jones says initial feedback from the paper industry on TIRS has been "good," he'll have a better feel for whether it will be effective when an actual field test is conducted. Other analysis techniques are also being considered by the paper industry at this time, which, McClelland admits, may actually prove to be better fits than TIRS.

"If that's the case, then there may be additional aspects of the paper-making process that can benefit from



the TIRS technology," says a confident McClelland, who adds that instead of using TIRS to analyze wood chips as they are going into the paper digestor, it might be better to conduct the TIRS analysis at the other end of the production process, where the paper is being manufactured by the paper machine. "We're already conducting tests on different paper coatings and paper processes to see how well our technique works," says McClelland.

And beyond the paper manufacturing-industry, McClelland and Jones are looking at adapting TIRS to meet specific needs of the glass industry. "We have a proposal to analyze the 'cure' of coatings on fiber optic cables," says McClelland. If not properly cured, the cables stick together and the coatings tear as the cables are being unwound from spools. "This amounts to a multi-million dollar problem for this industry," says McClelland, "and we hope there might be an opportunity for TIRS to also have some impact in this area."◆

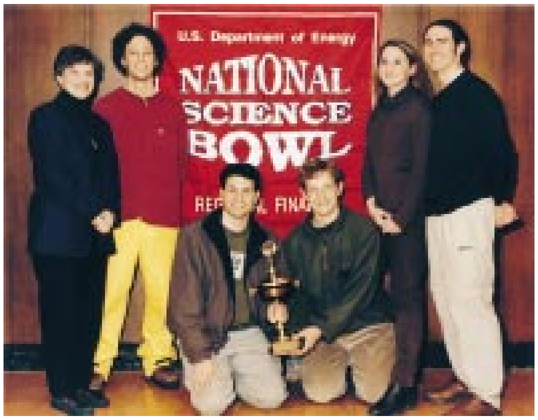
For more information:
Roger Jones, (515) 294-3894
jonesrw@ameslab.gov

John McClelland, (515) 294-7948
mcclelland@ameslab.gov

Current research funded by:
DOE Energy Efficiency and Renewable Energy Office

INtouch

Iowa-Grown Science Champs



A crackerjack student team from Valley High School in West Des Moines, IA, won the Department of Energy's 1998 National Science Bowl in Washington, D.C., in May. Valley progressed to the national competition after winning the Ames Laboratory regional competition in February.

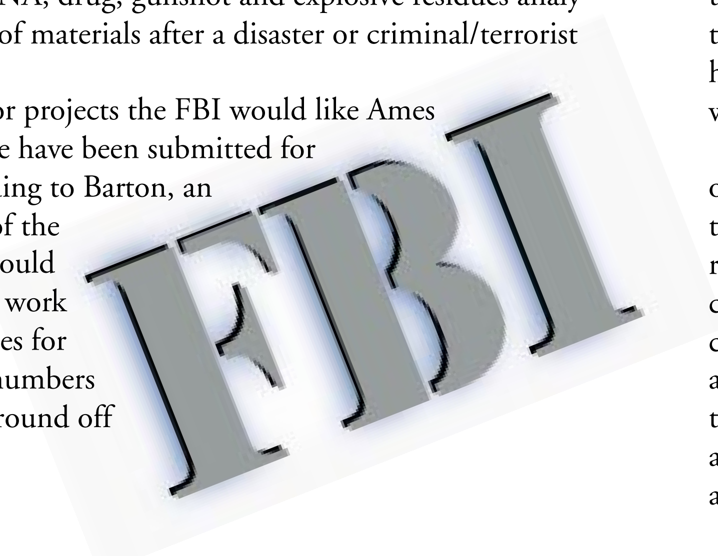
The science whiz-kids triumphed over 47 teams to capture the national championship. The Valley team received an all-expenses-paid trip to Lindau, Germany, to meet with Nobel Laureates in chemistry. During the one-week trip, they also attended a symposium with scholars from around the world.

Lab to Work with FBI

Ames Lab Director Tom Barton traveled to Washington, D.C., in May to witness the signing of a memorandum of agreement with the FBI and the Justice Department that will allow Lab scientists to tackle research for the FBI.

The FBI will draw upon the Lab's expertise in analytical methods and instrumentation development to help advance the frontier in forensic science. The FBI Laboratories make up the largest forensic science facility in the world. Scientists there are especially interested in portable and miniature analytical instrumentation for DNA, drug, gunshot and explosive residues analyses; and analysis of materials after a disaster or criminal/terrorist act.

Proposals for projects the FBI would like Ames Lab to investigate have been submitted for funding. According to Barton, an example of one of the things the Lab would do for the FBI is work on new techniques for analyzing serial numbers that have been ground off various items.



Ames Lab Wins DOE Award for Pretty Cool Stuff

The Department of Energy has recognized Ames Lab researchers Karl Gschneidner (above) and Vitalij Pecharsky for their contribution to the advancement of magnetic refrigeration technology. The two scientists were awarded the 1997 Materials Sciences Award for Significant Implication for Department of Energy Related Technologies in the Metallurgy and Ceramics category.

Gschneidner and Pecharsky discovered the giant magnetocaloric effect in gadolinium-silicon-germanium (GdSiGe) alloys, which are destined to boost the cooling power and efficiency of magnetic refrigerators. The magnetocaloric effect is the tendency of some metals to become hot when magnetized and cool down when demagnetized.

The high magnetocaloric effect of GdSiGe alloys not only improves the efficiency of large-scale magnetic refrigerators, making them even more competitive with conventional gas-compression technology, but may also lead to small-scale applications that include climate control in cars and homes, and in home refrigerators and freezers.