Oak Ridge National Laboratory

REVIEW

Vol. 31, Nos. 1 & 2, 1998

State of the Laboratory

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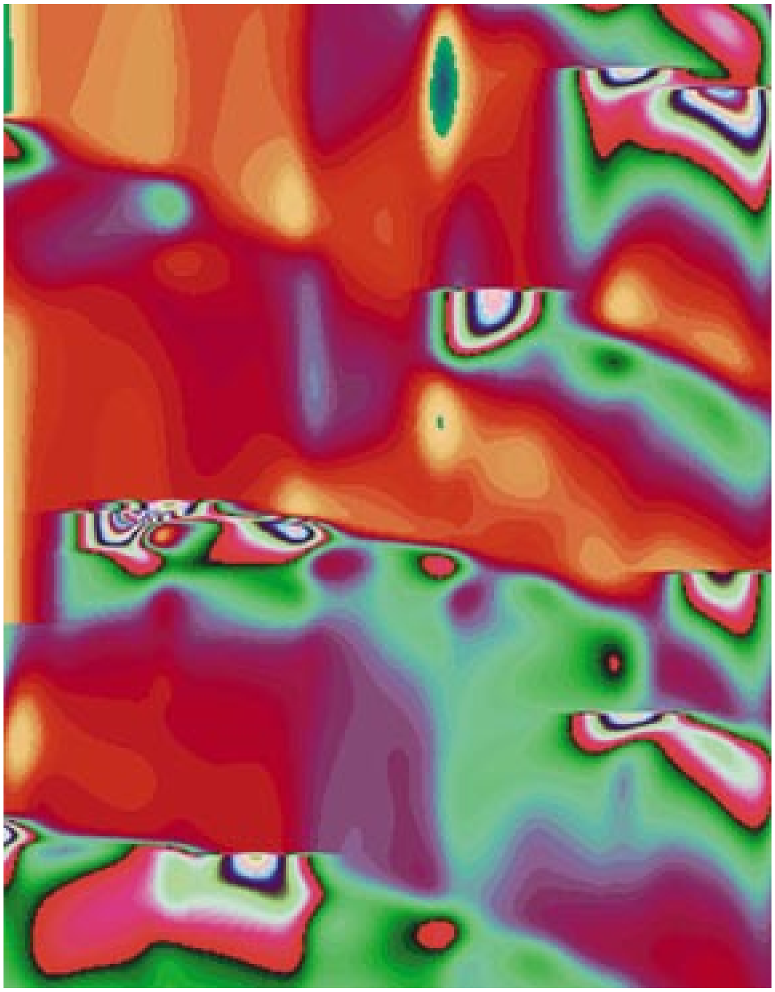

COVER CAPTION

Avalanches of particles and heat are imaged in a three-dimensional nonlinear computer model of turbulence in fusion plasmas. Research on "sandpile models" of plasma turbulence that leads to heat losses in fusion devices is described on p. 35. It is one of many science and technology projects in progress during 1997 and this year that are highlighted in this State of the Laboratory issue.

Oak Ridge National Laboratory is a multiprogram, multipurpose laboratory that conducts research in energy production and end-use technologies; biological and environmental science and technology; advanced materials synthesis, processing, and characterization; and the physical sciences including neutron-based science and technology.

REVIEW

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The *Oak Ridge National Laboratory Review* is published twice a year and distributed to employees and others associated with or interested in ORNL.

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Internet users can find the *Review* at: http://www.ornl.gov/ORNLReview/.

The *Review* is also available on microfiche at the ORNL Central Research Library.

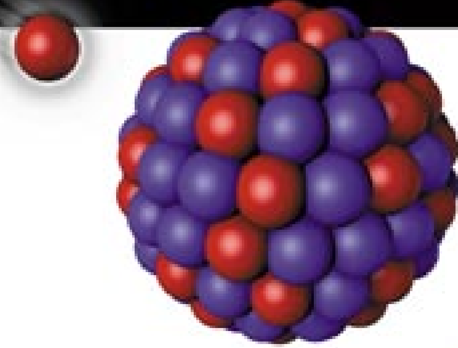
If you have changed your mailing address and want to remain on the mailing list, please notify the editorial office.

The *Review* is printed in the United States of America and is also available from the National Technical Information Service, U.S. Department of Commerce, 5285 Port Royal Road, Springfield, VA 22161.

ORNL is managed by Lockheed Martin Energy Research Corp. for the Department of Energy under contract DE-AC05-96OR22464.

ISSN 0048-1262

Produced by the Office of Communications and Public Affairs and the Computing, Information, and Networking Division.



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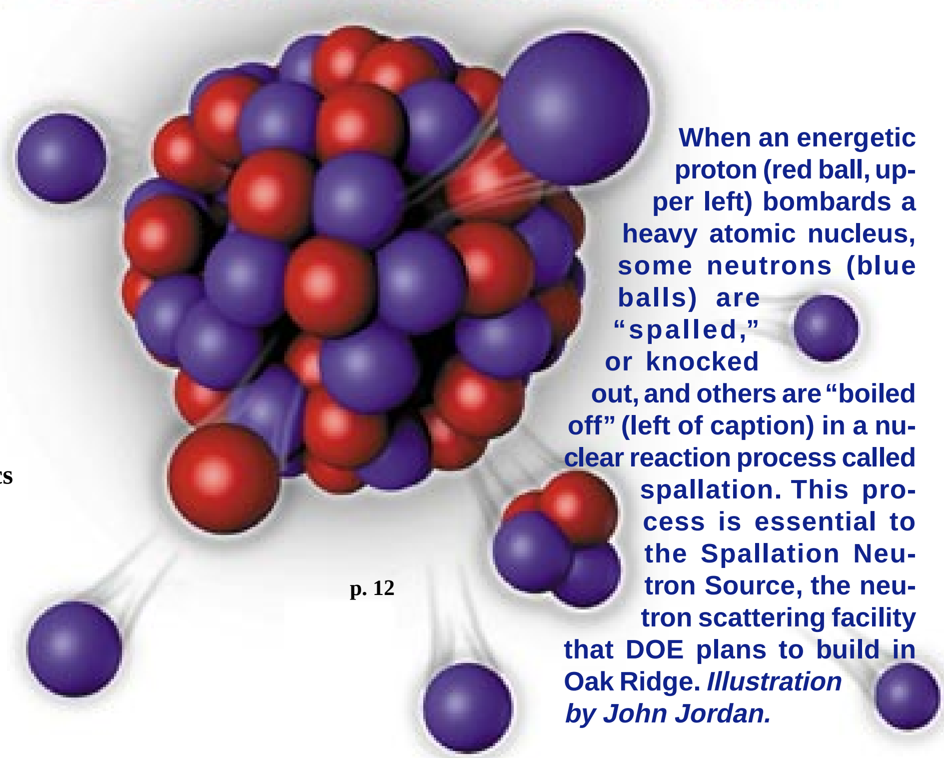

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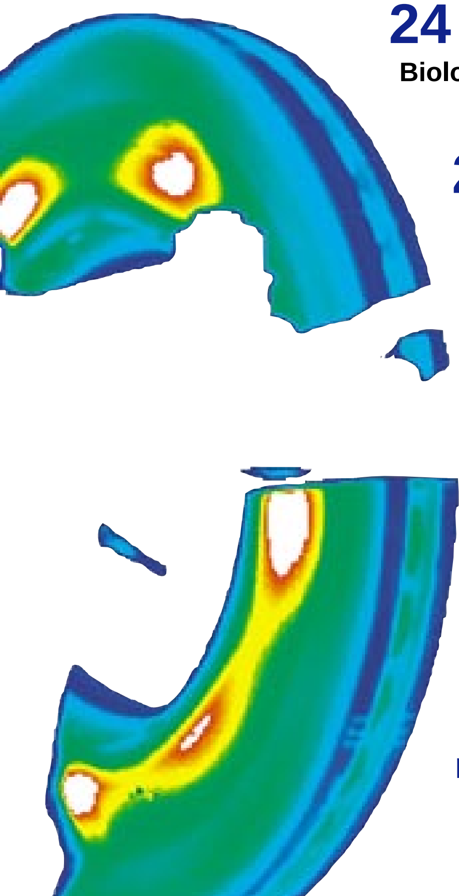
When an energetic proton (red ball, upper left) bombards a heavy atomic nucleus, some neutrons (blue balls) are "spalled," or knocked out, and others are "boiled off" (left of caption) in a nuclear reaction process called spallation. This process is essential to the Spallation Neutron Source, the neutron scattering facility that DOE plans to build in Oak Ridge. *Illustration by John Jordan.*



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ORNL's modified infrared camera has imaged hot spots on auto disk brake rotors that could lead to a better brake design and reduce the auto industry's warranty costs. This infrared snapshot shows hot spots on a rotor spinning at 60 miles per hour with the brakes applied.

Editor's note—ORNL Director Alvin W. Trivelpiece delivered his annual State of the Laboratory address to employees and guests on May 12, 1998, in Eugene P. Wigner Auditorium, Oak Ridge National Laboratory. An edited version follows.

State of the Labora

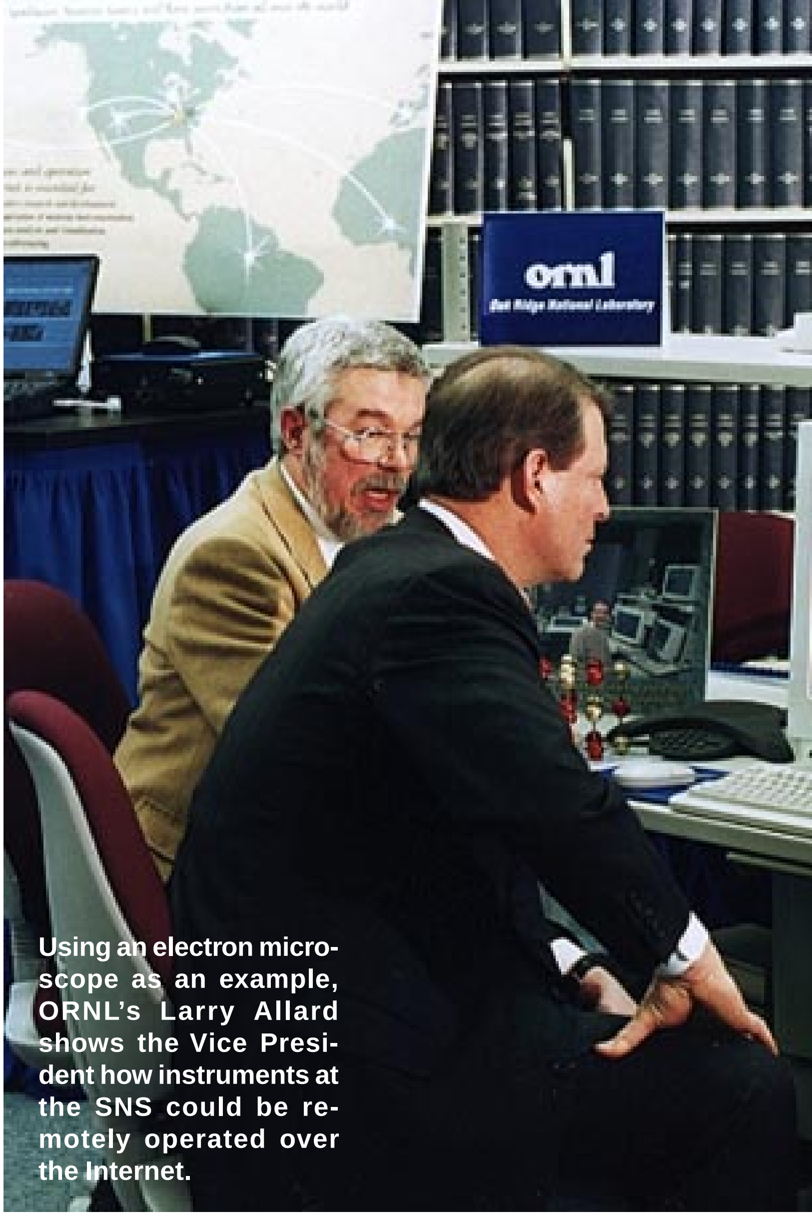
Vice President Al Gore's January 21, 1998, announcement about the Clinton administration's support for the Spallation Neutron Source (SNS) is received enthusiastically by, from left, Federico Peña, then Secretary of Energy; ORNL Director Al Trivelpiece; Tennessee Governor Don Sundquist; and William F. Brinkman, executive director of the Physical Sciences Research Division, Bell Labs, Lucent Technologies. ***Photograph by Tom Cerniglio.***

atory—1997

Opportunities and Challenges

ORNL's Herb Mook explains the value of neutron scattering to Vice President Al Gore.

ORNL Director Al Trivelpiece (second from left) shakes hands with Vice President Al Gore, who visited the Laboratory to announce the Clinton administration's proposal of $157 million for new construction funds for the SNS. Also present were Jim Hall (left), manager of DOE's Oak Ridge Operations; Bill Appleton, ORNL associate director for the SNS; and Knox County Executive Tommy Schumpert. *Photographs by Tom Cerniglio.*



Using an electron microscope as an example, ORNL's Larry Allard shows the Vice President how instruments at the SNS could be remotely operated over the Internet.

The opportunity for us is that the SNS is in the President's budget, and the challenge is to have favorable congressional action approving the project.

First, I would like to recognize Jim Hall, manager of the Department of Energy's Oak Ridge Operations Office, and to congratulate him on receiving a Presidential Rank Award for Meritorious Executives. In the past, I have been involved in the process of selecting winners for these awards. This is quite an honor, and it is given to only a few federal employees. The award includes a bonus for $10,000. Jim, when can we do lunch?

Second, I would like to recognize and congratulate Audrey Stevens, who was recently elected to the National Academy of Sciences. This is a singular honor that recognizes outstanding accomplishments.

Last year's State-of-the-Lab talk was given on June 12, so this is only an 11-month year. My talk will not be correspondingly shortened. A lot has happened in these last 11 months. I could devote the whole talk to describing the events of last year. However, I am not going to do that, but rather I am going to talk about some of the challenges that we face this next year, and I am going to talk about how we might take better advantage of the opportunities that are available to us. Even so, there are a few events from this past year that do seem worthy of some mention.

First and foremost was the announcement by Vice President Al Gore during his visit here on January 21, 1998, that President Clinton's FY 1999 budget would include a request for $157 million to initiate construction of the Spallation Neutron Source at Oak Ridge National Laboratory.

However, it is also important to remember that just because the President requests something doesn't mean that Congress is going to approve his request. The opportunity for us is that the SNS is in the President's budget, and the challenge is to have favorable congressional action approving the project.

Since the announcement that the funding to begin construction of the SNS would be in the President's budget was a pivotal

Vice President Al Gore hears from ORNL's Michael Wright how science can be conducted from a distance using computers and high-speed links between geographically separated laboratories.

event in ORNL's history, I would like to review a few of the events leading up to the moment of the Vice President's announcement.

Once upon a time, in a galaxy far far away, there was an Advanced Neutron Source project. Funding had been requested for this project in both 1994 and 1995. Congress did not approve funding for the ANS. The question was, should funding be requested a third time, or was our situation like the classic statement about drowning? Namely, if you go down for the third time, it's all over. In November 1994, we were given the opportunity to have the ANS put into the budget one more time. It was painfully clear that Congress was unlikely to approve such a request. At this same time, we were given less than one day to decide to stay with the ANS or to abandon it and switch to a Spallation Neutron Source. This was a difficult choice. After all, Congress might not approve initial funding for a Spallation Neutron Source at a level that would even permit doing a conceptual design for such a facility. Should we abandon the ANS or not? That was the question.

Our situation was somewhat like that of the worker on an oil platform in the North Sea that was on fire and about to explode. He was trapped out on the rig in a place that was over 100 feet above water. If he jumped and survived the fall, he was likely to die from hypothermia in just a few minutes. No rescue boat was in sight and he wasn't wearing flotation gear. Worse, there was a flaming oil slick on the water below him and a lot of debris floating in it. So even if he survived the fall, and didn't hit any debris, and didn't get burned in the oil fire, he still faced hypothermia. He jumped! It turns out that he was quickly rescued by the crew of a nearby boat, so he was one of the few survivors of this disaster. When asked later why he jumped, he said that if he had stayed on the platform, he faced certain death, but if he jumped, he faced only probable death. Well, if we had stayed with the ANS, it was certain death, but if we jumped to the SNS, it was only probable death. We jumped!

We had to start over and put together a team to prepare a new conceptual design report for a Spallation Neutron Source.

There was no rescue boat to pick us out of the cold water. We had to start over and put together a team to prepare a new conceptual design report for a Spallation Neutron Source. It was necessary to develop a new approach to building such a facility, because we didn't have the in-house experience in building accelerators of the sort needed for a spallation source. We had to defend ourselves against some of the other national labs that believed that they should have been selected to be the site for the SNS. Switching from the ANS to the SNS was not easy, but what is important is how we

responded to this new opportunity that came wrapped in a large challenge.

I am pleased and proud of the way that everyone involved quickly overcame his or her intense personal disappointment over the termination of the ANS and turned to the task of working on the SNS. A conceptual design report was prepared and defended. Without a suitable conceptual design, there couldn't be any administration support. It was also essential that a sound management plan be developed and accepted. None of these tasks was easy, there wasn't much time to get them done, and there certainly was not enough money to do them.

As I look back over time since we had to make that quick switch from the ANS to the SNS, I cannot help but admire the outstanding job Bill Appleton has done in leading this effort. He has worked hard and made many personal sacrifices to bring about the technical and managerial results that provided the Clinton administration with the confidence that a facility like the SNS can be built on schedule within cost—and that it will do what it is supposed to.

Without such solid hard work, it would not have been possible for Vice President Gore to have the opportunity to come here and announce that the SNS would be in President Clinton's FY 99 budget. Without such solid hard work, we would not have the essential support of the Department of Energy. Without such solid hard work, we would not have the $8 million pledged by Governor Sundquist as a cost-sharing contribution by the state of Tennessee for the SNS. These funds will build a much-needed facility near the SNS site to house the Joint Institute for Neutron Sciences. Without such solid hard work, it would not be possible to hope for the support of this project by the Congress.

I believe that we are executing our work much better now, but we have to be still more competitive as a national laboratory.

We still have a long way to go this year before we might have congressional approval for the SNS. There is no guarantee that such approval will occur and that funds will be appropriated to start the SNS. Fortunately, members of the Tennessee delegation have been very supportive of the SNS project. Without their help, it is unlikely that the SNS would be approved in the Congress. Therefore, I was really pleased that Congressmen Jimmy Duncan, Harold Ford, Jr., Bart Gordon, and Zach Wamp showed their support for the SNS by coming to ORNL with the Vice President when he made his announcement.

Without Bill Appleton's efforts, we would not have the unique arrangement for designing and building the SNS through a collaboration with four other national laboratories. They are Argonne National Laboratory, Lawrence Berkeley National Laboratory, Brookhaven National Laboratory, and Los Alamos National Laboratory. Obviously, a lot of people have helped Bill along the way and they deserve a fair share of credit for what they have accomplished. Even so, as I see it, Bill deserves our special thanks for the pivotal role that he has played in getting us from the ANS to the SNS. Please join me in thanking Bill.

Over the years I have had the privilege of assisting in making arrangements for several visits for appointed or elected officials to various places. Each such visit has its own special opportunities and challenges. A visit by the President or the Vice President presents an enriched opportunity for something to go terribly wrong and an enlarged chal-

On February 20, 1998, Al Trivelpiece signed a Mentor-Protégée Agreement with Advanced Integrated Management Services, Inc., whose president is Reggie Hall (seated left of Trivelpiece). This special event was the culmination of an ongoing process of identifying and solidifying a relationship between ORNL and a minority-owned business that would promote economic and technical growth and help to foster a long-term business relationship in support of DOE and ORNL missions. *Photograph by Jim Richmond.*

lenge to get it done right. It is necessary to be able to work with elected officials, the Secret Service, the advance team, speechwriters, special guests, dignitaries, caterers, painters, guards, and many others. Of all of these kinds of events that I have been involved in, the visit by the Vice President to ORNL was by far the best organized and executed. It couldn't have gone better. At the middle of it all was our own protocol officer, Nancy Gray. Nancy did an outstanding job of getting it all done with skill and grace under fire. Please join me in thanking Nancy.

I know that many of you were inconvenienced by the events leading up to the Vice President's visit. If you stood still anywhere in or near Building 4500 North for more than a few minutes, you were painted, swept, replaced, mopped, or mowed. I want to again thank all of you who did such a great job of painting, sweeping, replacing, mopping, and mowing to get the Lab in shape to receive our guests properly.

Why have I spent so much time talking about the Spallation Neutron Source Project? True, it is a large project and it certainly is important to the Lab's future. But this is not the reason. I want to use it as an example of what it means to be competitive. I am sure that all of you know the line from William Shakespeare's Julius Caesar. No, not, "Et tu Brute," but rather, "The fault, dear Brutus, is not in our stars, but in ourselves, that we are underlings."

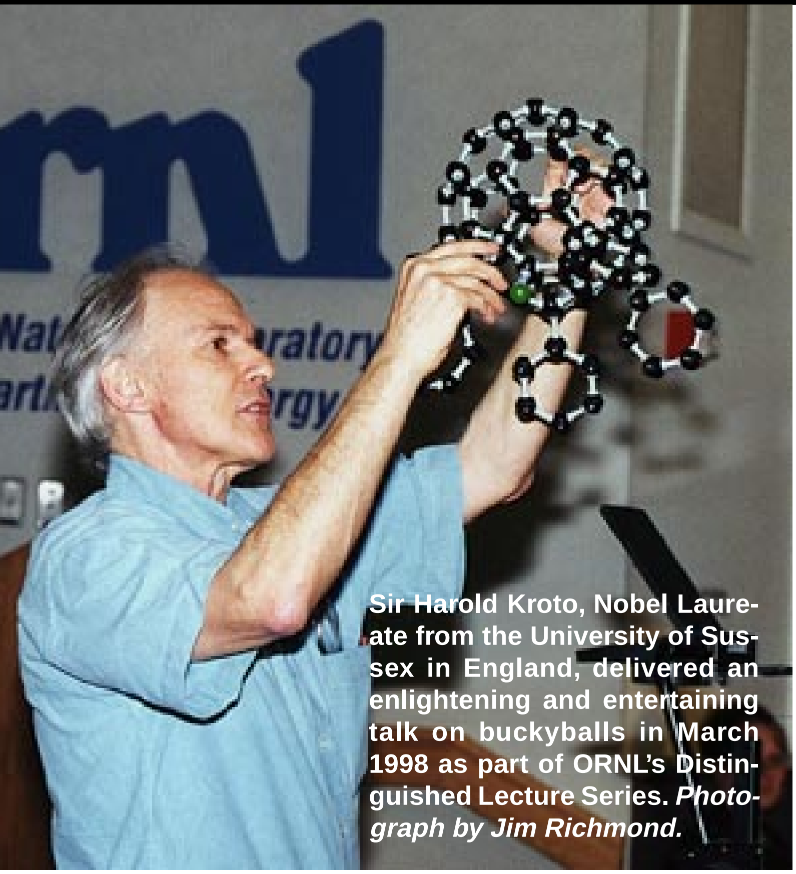
To me this is the essence of being competitive. That is, not to blame something or someone else for the fact that you didn't get what you believed was due you because of

ORNL will be the first national laboratory to give scientists and engineers the kind of financial tools that will permit more effective management of R&D programs.

your good looks, or the pivotal role that your institution played in the development of atomic weapons in World War II. Perhaps you didn't train hard enough to run fast enough to win the foot race. Perhaps your otherwise stellar proposal that didn't get funded contains an unfortunate number of avoidable spelling errors. You didn't get the job because. . . I will let you complete the list of reasons for failure from your own experiences. I always favored "the dog ate my homework." I guess the more modern version is "my hard disk crashed."

Because we have separated from Lockheed Martin Energy Systems (LMES), we no longer have the excuse that their business rules prevent us from doing whatever. After all, the rules we must follow are now our business rules. If they don't enhance our ability to compete, we should change them. That takes time and work, but it is not impossible. From time to time I hear that the weapons labs have an unfair advantage. That's true, but so what. I also hear that New Mexico has an unfair advantage because of its congressional delegation. Maybe, maybe not. If the SNS team had allowed themselves to consider the odds against getting as far as they have, they might well have just given up. They didn't. Their aggressive and competitive spirit should be more widespread at ORNL.

Right now we have a wonderful new opportunity with the Strategic Simulation Initiative (SSI). Earlier, the DOE weapons labs initiated an Accelerated Strategic Computing Initiative (ASCI) as part of their Science-Based Stockpile Stewardship program. DOE Under Secretary Ernie Moniz has decided to use the ASCI program



Sir Harold Kroto, Nobel Laureate from the University of Sussex in England, delivered an enlightening and entertaining talk on buckyballs in March 1998 as part of ORNL's Distinguished Lecture Series. *Photograph by Jim Richmond.*

Trivelpiece congratulates Marilyn Lloyd during the dedication of the Marilyn Lloyd Environmental and Life Sciences Complex. *Photograph by Manuel Gillispie.*

as a springboard to launch the SSI on a department-wide basis. Workshops were held to determine which technical areas would benefit from a major thrust to establish computing capability at the level of 30 to 100 teraops (trillions of arithmetic calculations per second). It was decided that the understanding of what influences climate change was a worthy subject. It was agreed that research into combustion using such computers could make a difference in emissions from internal combustion engines. It was proposed that the ability to design materials and to make progress in other scientific and technical fields are worthwhile goals. All of this is directed toward proposing that an element be added to the Department's FY 2000 budget to accomplish these goals. This would be a several-hundred-million-dollar program, if it materializes. That means submitting the request to the Department's budget by this June or July. All of this SSI effort is then directed ultimately at the President's signing the appropriation bills that would support such work into law in October 1999. A lot has to happen between now and then.

To get started on this effort, Under Secretary Moniz invited all of the directors of the Department's labs to a one-day meeting in Washington a few weeks ago. The SSI was discussed, and a program that would seek to make it happen was laid out. Martha Krebs, director of DOE's Office of Energy Research, and I were asked to chair a group that was assigned the responsibility of setting up an outreach program. This may involve having a conference in Washington in the near future. It will be a challenge to get this done. Are the chances that this initiative will lead to new DOE programs good? Maybe. We will not know if we don't try. Ed Oliver, our associate director for Computing, Robotics and Education, is on detail to the Office of Energy Research for a few months to help make this happen.

I am more optimistic this year than last about the future of the Lab.

When I hear how Sandia National Laboratories does as well as it does because of its political support, I have to smile. They write excellent proposals, they do a good job of marketing them, and they have a good sense of which areas might be in line for increased support by the government. Perhaps some of their success is related to the fact that they have more than 100 members of their staff in Washington on detail working in virtually every agency of our government. We are doing better in this regard, but we need a lot more people

Robert J. Stevens (right), president of the Lockheed Martin Energy and Environment Sector, chats with ORNL's Mark Spann. ***Photograph by Jim Richmond.***

I believe that new opportunities for funding in areas where ORNL could be expected to compete will increase. Our challenge is to find out where that funding is going to appear and then to write winning proposals.

like Ed Oliver working to make programs like the SSI come into being. We then need to write proposals that compete with places like Sandia. Now is the time to start writing proposals for the SSI, not a year from now. I have noticed a tendency here to wait until the money is in the budget and then assume that we will get a fair share. This may have worked in the past, but it sure doesn't seem to work too well today. I don't want to belabor the point and maybe I already have, but I want to make it clear that nobody is going to give us anything. We (you) have to write proposals that compete with those written by university faculty members. In fact, they have to be better proposals because there is a bias in funding agencies in favor of universities. Now that ought to get a rise out of somebody.

Last summer, President Clinton challenged his Cabinet to provide him with some information on what could be done to reduce greenhouse gas emissions. Secretary Peña in turn asked the directors of the Department's laboratories to conduct a study and write a report on this subject. Dick Truly, director of the National Renewable Energy Laboratory, and I were asked to lead this effort. We in turn asked Stan Bull and Dave Reichle to do the heavy lifting on this project. This effort involved coordinating the activities of nearly 200 scientists and engineers from 11 national labs. Dave was heard to mumble something about herding cats on horseback a few times. The report, which is widely known as the 11-Lab Study, is correctly titled Technology Opportunities for the Reduction of Greenhouse Gas Emissions. This report will not necessarily result in new opportunities for projects or programs at ORNL. However, if its recommendations are adopted, it should result in some research and development (R&D) programs in areas where ORNL should be able to compete. The challenge is to take the next steps that will cause programs to materialize. Dave and Stan did an outstanding job. This is the kind of activity that more members of our scientific and technical staff need to participate in if we and the other labs are to prosper.

Members of the Laboratory staff received directly or shared nine R&D 100 Awards in 1997 from *R&D* magazine. This is a record for ORNL, and the number of awards we won was more than any other DOE lab received. I took good advantage of the bragging rights the nine R&D 100 Awards gave us over some of our sister labs.

We also paused for a moment to thank our former Third District Representative, Marilyn Lloyd, by designating the west end of the Lab as the "Marilyn Lloyd Environmental and Life Sciences Complex." This is a well-deserved recognition for someone who has given much to ORNL and who continues to support our goals and objectives.

Professor John L. Finney, Quain Professor of Physics at University College in London, was hosted by Bill Appleton, ORNL associate director for the Spallation Neutron Source. Finney gave a talk at ORNL on scientific research that would be possible if the proposed European Spallation Source is built. *Photograph by Curtis Boles.*

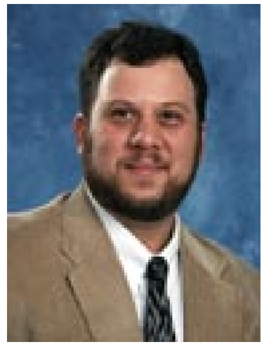
A conference on "Partnering for Functional Genomics Research," organized by ORNL, the University of Tennessee at Knoxville, and the Gene Research Access Corporation (GENRAC), was held at Pollard Auditorium. About 15 companies accepted the invitation to attend. It was a good event that resulted in the establishment of good contacts that may lead to some new opportunities for research on functional genomics. I also believe that we are on the path to a new facility for the mouse colony.

Together with the University of Tennessee we are working to bring into being a transportation research center to be located on Pellissippi Parkway. Secretary Peña presented a check for $870,000 during the Knoxville Summit to help get this project under way.

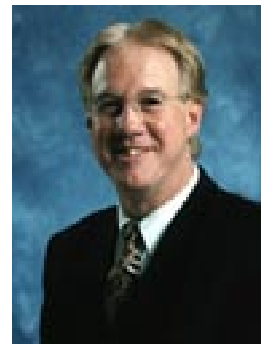
I would like to remind you that it was just a little over two years ago that ORNL was separated from LMES and that we were allowed to have a separate corporate structure better suited to our needs and functions. This was a great opportunity, and you have done much to take advantage of it. However, much remains to be done. Al Narath retired this year as the president of the Lockheed Martin Energy and Environment Sector, and Bob Stevens replaced him. These corporate comings and goings may not seem to have much direct influence on our daily activities, but they do have a major effect on the more global aspects of our activities. It was Al Narath who sought and obtained Department of Energy approval to have ORNL separated from LMES. Lockheed Martin Corporation has played an essential, but nearly invisible, role in the efforts that have resulted in the SNS being in the budget. Events such as the visit to Oak Ridge by Senator Pete Domenici and Senator Bill Frist don't just happen. Their visit was one of the keys to the SNS. That visit would not have occurred without Lockheed Martin help. I am pleased that Bob Stevens is following the same supportive approach for ORNL that Al Narath started. Narath will continue to serve as chairman of Lockheed Martin Energy Research Corporation's Board of Directors.

I am also pleased that Lockheed Martin continues to emphasize ethical behavior among its most important corporate goals. This year again, all of the nearly 200,000 Lockheed Martin employees will receive ethics training either from or with their direct supervisor. This is an important function. I have seen several companies nearly go bankrupt for failure to adhere to the highest ethical standards of behavior. Please take

One of our main challenges remains recruiting and retaining excellent scientists and engineers.





Clockwise: in 1998 Audrey Stevens was elected a member of the National Academy of Sciences for identifying and characterizing eight proteins. In 1997 David E. Newman and David J. Dean each received a Presidential Early Career Award for Scientists and Engineers. Jonathan Woodward received the Christopher Columbus Fellowship Foundation's $100,000 award for his new procedure that uses enzymes to produce hydrogen gas from simple sugars. Rodney McKee received a NOVA Award for Technical Excellence from Lockheed Martin Corporation in 1997 for the development of a transistor that will allow computer memory chips to hold more information and enable users to read and write on them faster. The development of short superconducting tapes using textured substrates received a NOVA Award for Teamwork from Lockheed Martin Corporation in 1997. Team representatives who were honored were, from left, Mariappan Paranthaman, Dave Christen, and Don Kroeger.

your ethics training seriously. I do. In addition, Lockheed Martin conducts an ethics survey every few years to provide us some information on how we do in this area with respect to other Lockheed Martin organizations. The ethics survey reveals some areas where we need to better understand what the answers mean and to take appropriate action.

It was this separation from LMES that gave us the chance to have a reengineering program. It has not gone as fast in producing results as many of you would like, or me either for that matter, but I would remind you we have only been at this for a little over two years. Other organizations with resources and flexibility that greatly exceed ours take many years to complete their programs. The new SAP accounting system is expected to be in operation in October 1998. With it, ORNL will be the first national laboratory to have put into the hands of its scientists and engineers the kind of financial tools that will permit more effective and efficient management of research and development programs. This should make you more competitive. It is a good opportunity. Your challenge is to take advantage of it.

The various human resources reengineering projects are doing well. There is a lot of work yet to do, and some of these activities take more time. Even so, the new approach to salary administration is providing many of you with better tools with which to run your programs.

One of our main challenges remains recruiting and retaining excellent scientists and engineers and all of the other talented people it takes to make a national laboratory. We need to do this in a way that recognizes the need to be a diverse organization. We need to do this during a period of great uncertainty as we adjust to working with Bechtel Jacobs.

Last year I mentioned that Richard Genung had volunteered to set up a program called Leadership ORNL. It is modeled after community leadership programs. This activity is going well.

There are many other subjects that I might have discussed today, but none of them would have changed my principal conclusions about the state of our Laboratory. Namely, that in spite of all of the uncertainties that we face, I am more optimistic this year than last about the future of the Lab. I believe that new opportunities for funding in areas where ORNL could be expected to compete will increase. Our challenge is to find out where that funding is going to appear and then to write winning proposals. For those that we win, we need to perform the work in an excellent and cost-effective manner. I believe that we are executing our work much better now, but we have to be still more competitive as a national laboratory. I look forward to being able to tell you next year about the progress that has been made on constructing the SNS.

Yevgeni P. Velikhov, president of the Kurchatov Institute in Russia, gave a talk on the future of energy development in February 1998 as an ORNL Distinguished Lecture.

♦ AWARDS ♦

Trivelpiece Presents Laboratory Director's Awards

The ORNL Award of Excellence in Environment, Safety, and Health recognizes distinguished and outstanding performance in the area of environment, safety, and health (ES&H) by any ORNL division or program during the previous calendar year. By giving this award, we emphasize the importance that ORNL places on this area of our activities. This year's award goes to the Chemical and Analytical Sciences Division.

The citation reads: "For exemplary teaming to achieve sustained superior ES&H performance, for an effective self-assessment program, for cost-effective pollution prevention initiatives, and for leadership in Laboratory-wide ES&H activities." Accepting the award was Marvin Poutsma, division director.

The ORNL Award of Excellence in Operations and Support recognizes distinguished and outstanding performance by an operations and support division or program during the previous calendar year. By giving this award, we emphasize the importance that ORNL places on providing the kind of service that will make us more competitive. This year's award goes to the Technical Support Section of the Instrumentation and Controls Division.

The citation reads: "For outstanding and dependable maintenance of the Laboratory's electronic instruments, for recognized customer service and satisfaction, for dedication to quality and efficiency, and for contributing as integral team members to ORNL's research teams." Accepting the award were Dan McDonald, division director, and Richard Hess, section head.

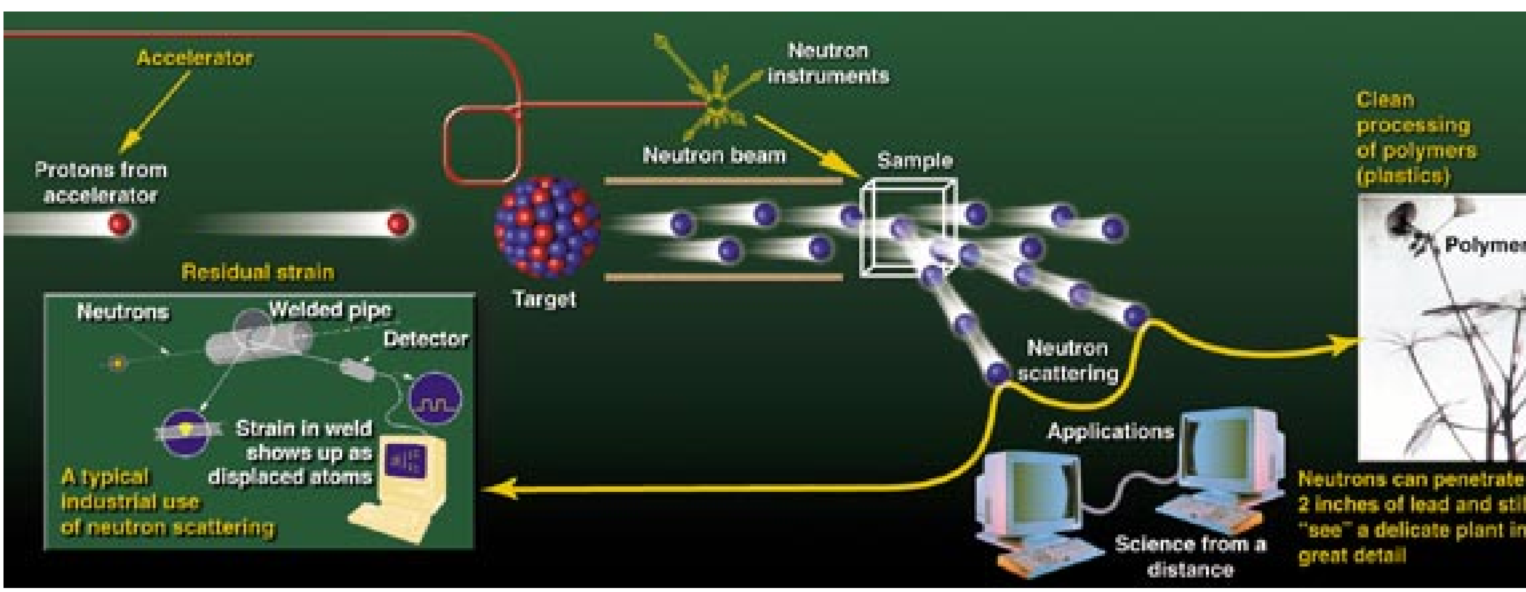
The ORNL Award of Excellence in Research and Development recognizes distinguished and outstanding performance by a research and development division or program during the previous calendar year. By giving this award, we emphasize the importance that ORNL places on excellence in research and development, which is at the core of our reason for existence. This year's award goes to the Metals and Ceramics Division.

The citation reads: "For recognized leadership in materials R&D at ORNL, in the United States, and in the international community, and for outstanding leadership within ORNL in the areas of reengineering, cost-effectiveness, ESH&Q, and work force diversity." Accepting the award was Linda Horton, deputy director of the division.

On October 10, 1997, ORNL dedicated the Marilyn Lloyd Environmental and Life Sciences Complex. The complex is named in honor of retired U.S. Representative Marilyn Lloyd, who served Tennessee's 3rd District, which includes Oak Ridge. Among the dignitaries participating in the dedication ceremony are, from left, Trivelpiece; U.S. Representative Jimmy Duncan of Tennessee's 2nd District; ORNL's Liane Russell, senior corporate fellow in the Life Sciences Division; Martha Krebs, director of DOE's Office of Energy Research; former Tennessee Representative Marilyn Lloyd; U.S. Representative Zach Wamp of Tennessee's 3rd District; Herman Postma, former ORNL director; and Gordon Fee, former president of Lockheed Martin Energy Systems. ***Photograph by Curtis Boles.***

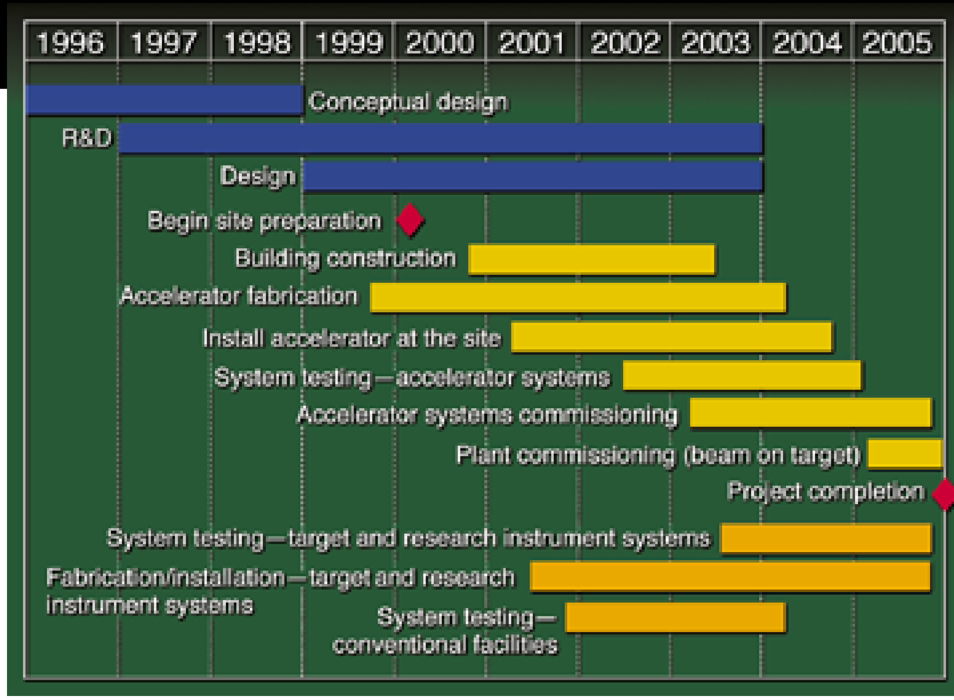
The Spallation Neutron Source: The Nation's Next-Generation Neutron-Scattering Facility

The Spallation Neutron Source (SNS) is an accelerator-based, next-generation neutron-scattering facility scheduled to be built on the Oak Ridge Reservation. Because it will produce more neutrons per second for a given area than any other neutron source, the greater brightness of the SNS will enable researchers to "see" never-before-observed details of physical and biological materials, ranging from plastics to proteins. The SNS is the top-priority project of the U.S. Department of Energy's Office of Energy Research (DOE-ER), which already has committed $39 million for its design and preparation. It will produce neutrons by bombarding a mercury target with energetic (1000-million-electron-volt) protons. The protons will excite the mercury nuclei, knocking loose and boiling off neutrons through a nuclear reaction process called spallation. The performance require-



ments and instrumentation needs of SNS are being determined in close collaboration with the scientific user community, and SNS will serve 1000 to 2000 users each year when completed. The project's total cost is estimated at $1.3 billion, and its construction is scheduled for completion in 2005.

The SNS project began in FY 1996, when DOE-ER directed ORNL to initiate research and development (R&D) and conceptual design studies. To carry out these studies in a timely and cost-effective manner, ORNL entered into a collaborative arrangement with four other national laboratories: Argonne, Brookhaven, Lawrence Berkeley, and Los Alamos. This SNS Collaboration, which will continue through the project's construction and operation, uses DOE's best technical expertise and newest technologies, as well as its vast experience with user programs involving scientists and engineers from universities, industry, government laboratories, and foreign institutions.

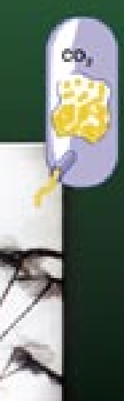


Schedule for the Spallation Neutron Source Project.

The SNS Collaboration completed its conceptual design report (CDR) in May 1997. In June 1997, a team of 65 external reviewers organized by DOE-ER held a week-long, comprehensive analysis of the CDR. The reviewers strongly endorsed the SNS Collaboration, its reference design, technical scope, cost, schedule, and collaborative-management approach. Moreover, the SNS Collaboration's estimate of the total project cost was within 1% of the estimate made by an independent cost-estimation team composed of representatives from industry.

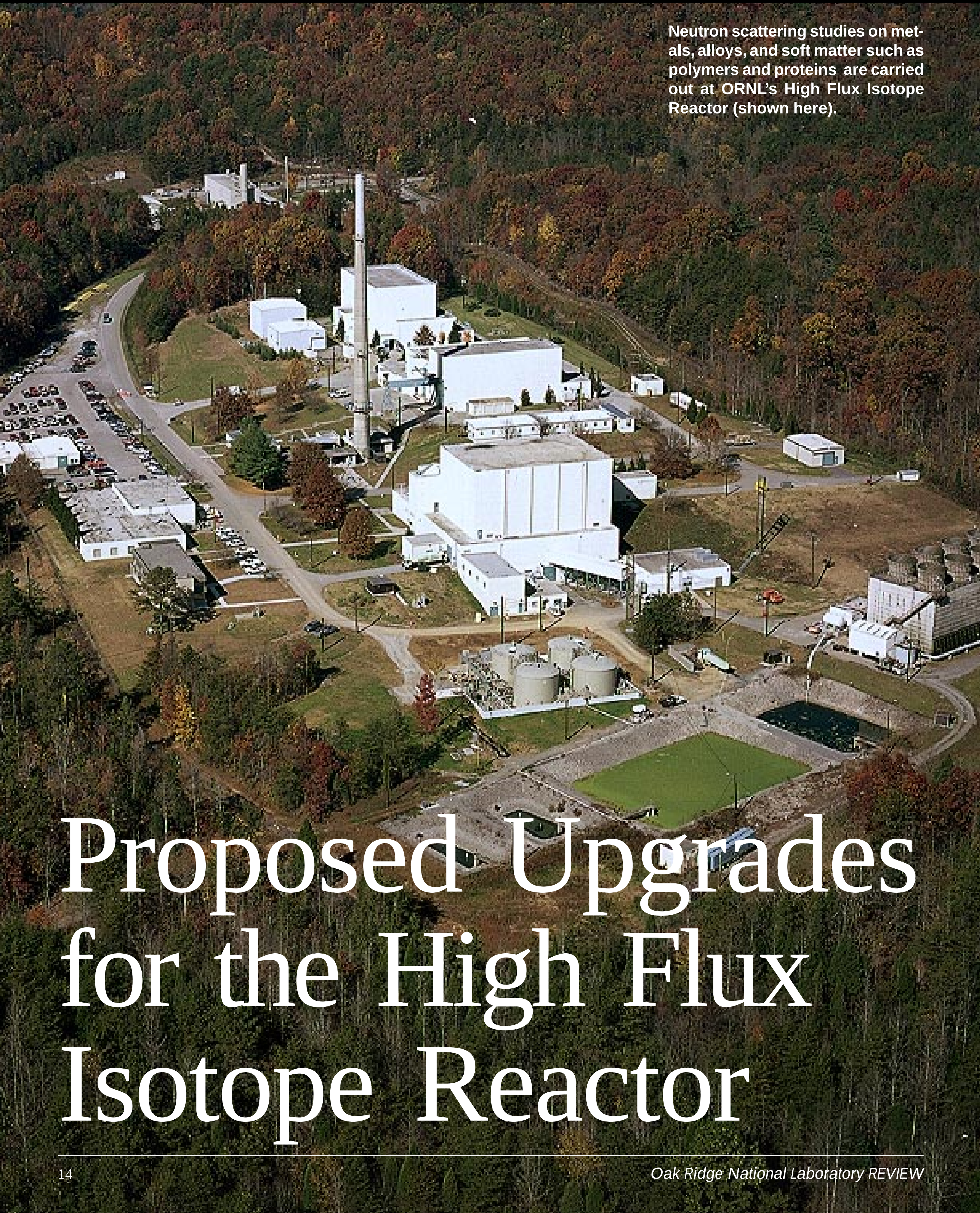
On January 21, 1998, Vice President Al Gore came to ORNL to announce that the Clinton Administration had made a construction line item request of $157 million for the SNS in its FY 1999 budget, which must be approved by Congress. At the announcement ceremony, Gore said, "I'm really delighted to be here at ORNL, the birthplace of neutron-scattering science, to make an announcement that will reclaim America's position as the world leader in a technology that we Americans invented." The SNS Collaboration will provide funds it receives from DOE to instrument 10 beam lines, and the instruments will be selected and built by the scientific community. Neutron scientists and technicians will be on hand to assist the user community once the instruments are completed. Eight more beam lines will be available for special instrumentation and collaborative access teams. The SNS is also designed to be upgraded economically to significantly higher power levels in the future.

The state of Tennessee, through the University of Tennessee, has committed $8 million for the establishment of the Joint Institute for Neutron Sciences (JINS). This new institute will serve as the gateway for the 1000 to 2000 guest scientists and engineers expected to come to East Tennessee each year to use the SNS and the nearby High Flux Isotope Reactor (HFIR), which is being upgraded (see following article). Because the upgraded HFIR will provide the most intense steady-state neutron beams and SNS will produce the most intense pulsed neutron beams for R&D anywhere, and because of the presence of JINS and other neutron-science capabilities at ORNL, Oak Ridge will be the world's leading center for neutron scattering research. *—Bill R. Appleton, ORNL associate director for the Spallation Neutron Source*



What Is Neutron Scattering and Why Is It Useful?

Because neutrons carry no net electrical charge, they interact only with the atomic nuclei of a material and can penetrate to far greater depths than charged particles, light, or even X rays without destroying the material. Thus, neutrons are extremely useful probes of matter in a neutron-scattering experiment. In such an experiment, a well-characterized beam of neutrons is directed onto the material under investigation. Some of the neutrons in the beam pass through the target material while others interact with the material and scatter from its nuclei. By measuring the angles, energies, and other properties of the scattered neutrons, scientists can obtain information about a material's structure and the motions of its atoms. This technique has been used to study fundamental properties of a wide variety of materials and to guide the development of products ranging from cars to computers, paints to plastics, new time-released medicines, and life-saving bulletproof vests. Thus, even though neutron scattering is not a household term, it plays a significant role in our lives by improving many of the products we encounter every day. *Illustration by Allison Baldwin.*



Neutron scattering studies on metals, alloys, and soft matter such as polymers and proteins are carried out at ORNL's High Flux Isotope Reactor (shown here).

Proposed Upgrades for the High Flux Isotope Reactor

ORNL's High Flux Isotope Reactor (HFIR) provides the highest thermal neutron flux in the western world. This unique facility is a national resource with missions in five important areas: transplutonium radioisotope production, high-specific-activity radioisotope production, neutron-scattering research, neutron activation analysis, and irradiation testing of materials.

The reactor was originally designed and used primarily to produce the transplutonium isotopes—elements beyond plutonium in the periodic table of elements, which do not occur naturally on earth. However, over time, the neutron scattering mission has grown in scientific and economic importance—providing, for example, experimental capabilities to more than 200 outside users per year.

The DOE Office of Energy Research and the Advanced Materials Physics and Neutron Sciences Directorate at ORNL are seeking to ensure that this versatile facility remains on the forefront of neutron science at the beginning of the next century. To do this, ORNL is taking advantage of a routine outage for replacing HFIR's permanent beryllium reflector to modify several components. This six-month reactor outage, which occurs about every 10 years, is currently scheduled to begin in late 1999. The package of upgrades will enhance our capabilities in all the mission areas, but the biggest impact will be on neutron scattering.

The HFIR design includes four horizontal beam tubes, designated HB-1 through HB-4, that supply streams of neutrons to the HFIR beam room where experimenters perform neutron scattering experiments using an array of specialized instruments. The HFIR beam tubes were designed and installed in the early 1960s when neutron scattering was in its infancy. The proven beam tubes are being modified to incorporate current technology. These modifications include

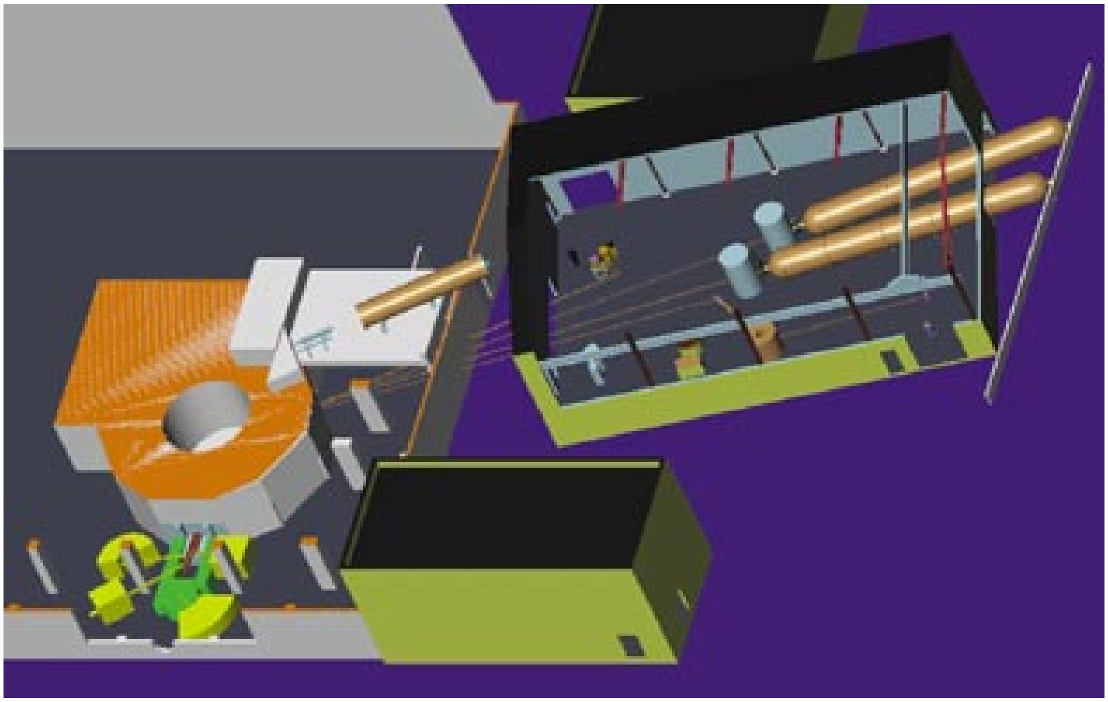
- Larger-diameter beam tubes that deliver more neutron flux to the neutron scattering targets
- Special beryllium inserts in the HB-2 beam tube designed to maximize the number of thermal neutrons entering an array of five new supermirror neutron guides
- A cold neutron source in the HB-4 beam tube which uses supercritical fluid hydrogen to slow down neutrons so they have very low energies and long wavelengths for experiments involving large molecules such as polymers.

The HFIR neutron scattering equipment and instrumentation is also being upgraded to the state of the art to take advantage of the improved neutron source provided by the reactor modifications. These improvements include new supermirror neutron guides on the HB-2 thermal neutron beam, new cold neutron guides for the HB-4 cold neutron beam, new monochromator crystal assemblies, and an array of new instruments, such as a 40-meter small-angle neutron scattering instrument and neutron reflectometer.

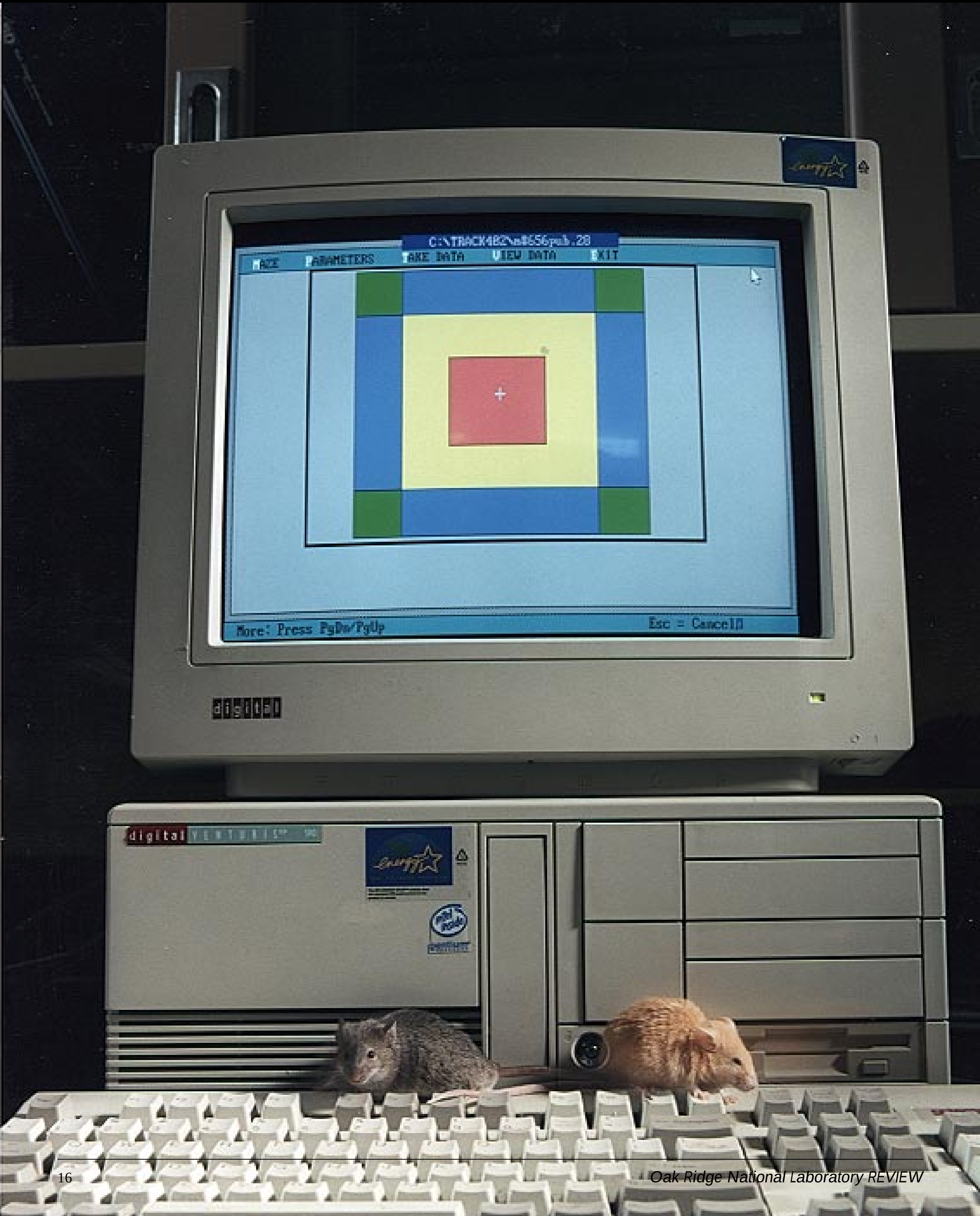
One of the most important tasks in this project is not a modification but, rather, a thorough analysis to verify that the HFIR vessel will remain sound well into the next century. Preliminary calculations show that the vessel can support safe and reliable reactor operation through 2035. This predicted longevity makes these modifications attractive to DOE and the neutron sciences community. The project will allow HFIR to provide world-class neutron sciences research facilities for many years to come.

In addition to these projects is a proposal to return HFIR to the original 100-megawatt design power level instead of the 85-megawatt level that has been used since 1989. This change will benefit all missions, because the neutron production rate, which is proportional to reactor power, will be increased by nearly 20%.

The HFIR is already the best reactor in the western world in thermal neutron flux, and these planned upgrades should make it even better.—*Colin West, HFIR Scientific Facilities Upgrade Project manager*



Proposed new instruments for the High Flux Isotope Reactor upgrade will increase the intensity of neutrons from the reactor but slow them down considerably. Such cold neutrons are needed to better evaluate the structure of polymers and proteins. *Digital image by Danny Williams.*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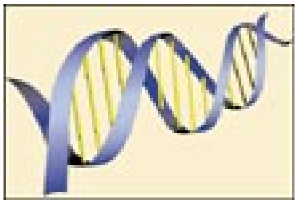
Functional Genomics

Large-scale human genome sequencing now under way is expected to produce several million base pairs every month for the next 5 to 10 years. This major effort will provide the biomedical research community with a computerized catalog of the names, locations, and nucleotide sequences of the 80,000 to 100,000 genes on human chromosomes. Based on the rate at which sequence data are being produced, some 75 new human genes could be discovered every day. Significant advances are required in our ability to determine the function of these genes to unlock all the information hidden in the output from sequencing and gene searches. Biologists have been studying gene function for many years, but most of their research has been slow, costly, and directed at single genes. Access to the powerful reagents from the genome program is changing all of this. In this new era of biomedical research, in addition to studying the function of individual genes, it will be possible to perform experiments in functional genomics—gene function on a genome-wide scale.

Gene function is determined by (1) analyzing the effects of DNA mutations in genes on normal development and health in the whole organism, (2) analyzing a variety of signals encoded in the DNA sequence, and (3) studying the proteins produced by a gene or system of related genes. Functional genomics at ORNL is a comprehensive effort that leverages strong expertise and facilities in mammalian genetics, bioinformatics and computational biology, and biochemistry, as well as the Laboratory's resources for structural biology and cutting-edge technology development. Functional genomics in humans is becoming tractable by using genome information from other model organisms that provide rich scenarios for experimental research.



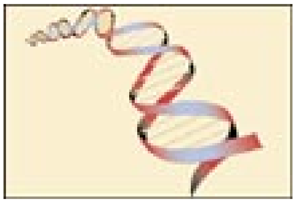
Mouse Genetics Research Facility

The mouse, because of its genetic and physiological similarities to the human and its extensive comparative genetic linkage map, is one of the leading model organisms for determining human gene function. A wide variety of genetic and molecular manipulations are possible in the mouse, making it a powerful research organism for studies of functional genomics. Mouse geneticists may "target" a specific gene to eliminate or alter its function in the whole animal or only in a specific cell population. They may add normal genes to a mutant mouse to correct an abnormality. They can engineer rearrangements in large regions of the genome and then create mutations gene by gene in the region using the chemical mutagen ethylnitrosourea (ENU) to make single-base changes in DNA. ORNL's Bill Russell discovered that ENU is a "supermutagen" and established the parameters for its effective use in mutagenesis experiments in the mouse. ENU has proven quite useful for making multiple mutant forms of a single gene, thereby providing more exact human disease models that mimic the subtle genetic variations characteristic of human populations. These strategies for creating mutations in mice can easily be expanded to a genome-wide scale, generating genetic reagents essential for the entire research community.

Just as you rarely see a computer without a mouse, you rarely see mice on a computer keyboard—a symbol for computational biology. *Photograph by Tom Cerniglio.*

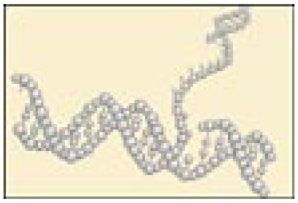
ORNL's Laboratory for Comparative and Functional Genomics, formerly called the Mouse Genetics Research Facility, represents one of the largest facilities in the world for carrying out experimental research in functional genomics using the mouse as a model organism. This newly designated DOE user facility currently houses some 90,000 mice representing a variety of mutations.

Mitch Doktycz checks the alignment of a robot's dispensing probes as he prepares to construct a set of flow-through genosensors. The dispensing probes transfer DNA sequences from microtiter plates to individual wells of the genosensors. Each genosensor measures less than half an inch on a side and contains almost 100 wells. A potential use of flow-through genosensors is rapid detection of genetic disease and other mutations. *Photograph by Tom Cerniglio.*



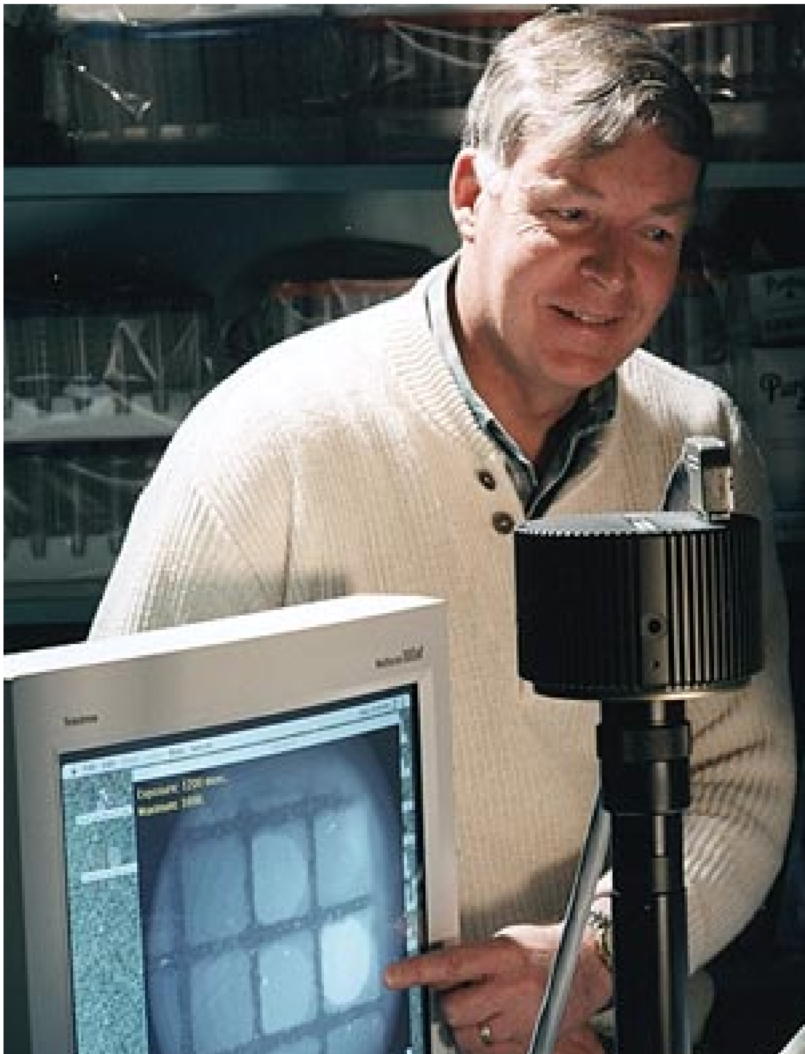
Bioinformatics Resource

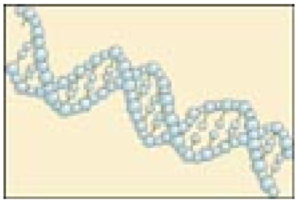
Since 1989, ORNL has been developing a bioinformatics resource for the genome research community, starting with the DNA pattern analysis system called the Gene Recognition Analysis Internet Link (GRAIL™). GRAIL™ is a suite of tools designed to provide analysis of DNA sequences both interactively and through the use of automated computation. The capabilities of GRAIL™ are available by several methods, including an electronic mail server at ORNL that processes DNA sequence(s) contained in e-mail messages, and an interactive graphical X-based client-server system called XGRAIL™, which supports a wide range of analysis tools such as gene modeling. The ORNL genome informatics resource is being used by thousands of researchers worldwide. ORNL informaticists and computational biologists lead the Genome Annotation Consortium, a collaborative effort involving several bioinformatics groups that work toward providing the analysis tools, information access, and processing environment appropriate to manage effectively the enormous amounts of data produced by large-scale genome sequencing.



Protein Analysis

Another critical component of the functional genomics research program at ORNL is the ability to quickly characterize the structure and function of the proteins that genes encode. This analysis involves a comprehensive effort to integrate protein engineering and enzymology, mass spectrometry, neutron-based structural biology, and computational approaches to the prediction of protein structure and function based on structure.

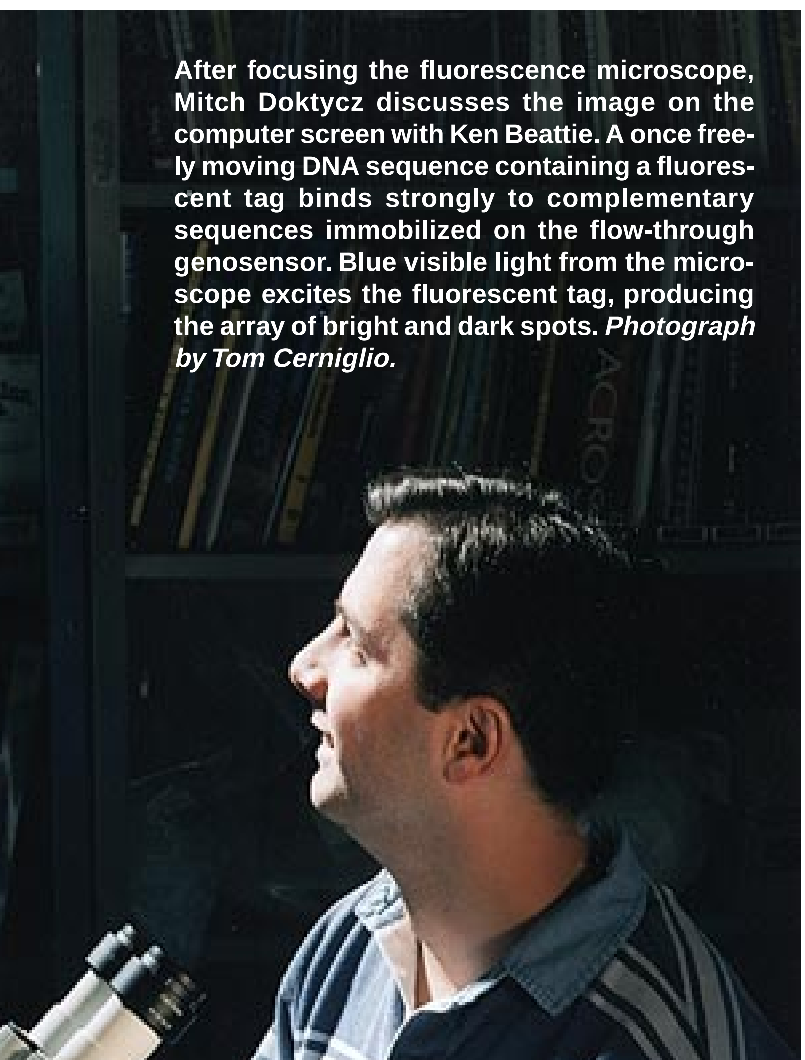




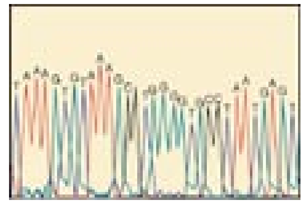
High-Throughput Analysis and Screening Systems Development

The large number of genes to be analyzed and the extraordinary complexity of analyzing the function of a system of genes and their interrelationships make it necessary to develop high-throughput technologies that can lead to truly genome-wide determination of gene function. The ORNL program includes a number of technology-oriented efforts that include flow-through genosensor-type chip arrays, fast DNA analyses employing the "lab-on-a-chip" concept, and other microinstrumentation developments for genome analyses.

This comprehensive effort is now in the second year of a three-year start-up period supported by ORNL's internally funded Laboratory Directed Research and Development Program. The team of researchers includes members of ORNL's Life Sciences, Chemistry and Analytical Sciences, Instrumentation and Controls, and Robotics and Process Systems divisions.



After focusing the fluorescence microscope, Mitch Doktycz discusses the image on the computer screen with Ken Beattie. A once freely moving DNA sequence containing a fluorescent tag binds strongly to complementary sequences immobilized on the flow-through genosensor. Blue visible light from the microscope excites the fluorescent tag, producing the array of bright and dark spots. *Photograph by Tom Cerniglio.*



Selected First-Year Achievements

Several key milestones have been met during the first year of ORNL's Functional Genomics Program. Efforts have resulted in the establishment of new programs in ENU mutagenesis and the testing of potential mutants for changes in behavioral and biochemical parameters. To date, behavioral aberrations in four existing mutant strains of mice have been documented for publication by Dabney Johnson's mammalian genetics laboratory, and 176 new litters have been screened for induced mutations in a large segment of mouse chromosome 4. ENU was used by Monica Justice to generate multiple alleles at two mouse loci involved in immune function. New recessive alleles of each locus were obtained, and eight new dominant mutations with relevant human disease phenotypes have proven to be heritable. These dominant mutations include ones that cause anemia, craniofacial abnormalities, neural tube defects, skin disorders, and cataracts.

Under Ed Michaud's direction, the transgenics laboratory has developed more efficient molecular systems for creating made-to-order mutations in specific genes or regions of the genome. Researchers in ORNL's Instrumentation and Controls Division are developing new technologies to automate screening techniques that are currently bottlenecked by a reliance on manual testing protocols. A database cataloging the entire Oak Ridge collection of mutant strains was created to make available information about the genes and genome regions in the mouse as research tools for the research community. The database has a Java interface so users can view the deletion complex and the mouse function data and make correlations and comparisons with human data.

An online resource about mouse mutant strains at ORNL was made available. Genome sequences become meaningful and useful if the information they contain is found, extracted, made explicit, and made accessible to the research community. The Genome Channel is a unique information resource and Web browser that gathers the distributed output of sequencing centers and provides a fully assembled view of the human genome, its chromosomes, clones, sequences, and experimentally known and computationally predicted genes. The initial version of the Genome Channel was well received at its debut at the 1997 DOE Genome Contractor's meeting in Sante Fe, New Mexico, by both the user community and sponsors. It is being developed by the ORNL-led Genome Annotation Consortium, whose mission is to bring biological meaning to the DNA sequence output of the Human Genome Project. This research tool captures sequence as it is generated worldwide, analyzes the sequence for new genes, and makes the information accessible to the genome community via the Genome Channel Browser. This work also addresses the development of a system that uses the World Wide Web's intelligent agents to dynamically locate and link to remote information about the function of known genes.—*Reinhold Mann, director of ORNL's Life Sciences Division*

ORNL's Path to Teraops Computing

In January 1995, ORNL had the fastest parallel supercomputer in the world—the Intel Paragon XP/S 150. It would run for less than a day at a time, but it was the only tool available for performing the most complex calculations of the day. By partnering with Intel, the staff of ORNL's Center for Computational Sciences (CCS) turned this and another Paragon into reliable supercomputers. These machines rapidly perform calculations to help scientists better understand complex phenomena, such as the movements of pollutants in groundwater and of particles in a gas, effects of growing atmospheric concentrations of carbon dioxide on future climate, and the behavior of materials ranging from melting to magnetism.

In the past four years, the reliability of the Intel Paragons has been strongly improved, stamping the CCS as a major Department of Energy (DOE) computational development center. However, largely because the speed of processor chips continues to double every 18 months (as predicted by Moore's law), the position of the Intel Paragon XP/S 150 in the hierarchy of powerful machines has slipped to #24. Our Intel Paragon XP/S

The SRC-6 is a machine of an innovative architecture being built by a company started by Seymour R. Cray. It will be installed at ORNL in 1998 for evaluation. *Model rendering by Ross Toedte.*

150, which once led the world in computing speed, can perform 150 billion calculations per second. But this multigigaops computer has been eclipsed by the superb Intel Teraflops machine at Sandia National Laboratories (SNL) in Albuquerque, which reliably provides a peak computing level near two teraops—trillion operations (arithmetic calculations) per second. The Intel Teraflops computer is used for classified defense work. SNL also has an Intel Paragon, which has been linked by a high-speed network data line to the ORNL Intel Paragons to leverage the ability of the three computers to solve complex problems in energy, environmental, and materials research.

New Strategy

Recent technological advances, the decision by Intel to halt production of new supercomputers, and the realization that our Intel Paragons have a limited lifetime and limited appeal to computational scientists looking for the fastest machines has compelled a new perspective. ORNL has decided to pursue a different path to achieving a teraops level of computing. This path will continue to offer challenging opportunities for CCS as a computational development center.

We have received DOE funding to purchase and install in 1998 a new parallel supercomputer built by SRC Computers, Inc., the company Seymour R. Cray (the inventor of the Cray supercomputer) was heading at the time of his death. Our plan is to evaluate comprehensively the performance of this machine, called the SRC-6. We hope to incorporate it into ORNL's collaboration with SNL on the networking of high-performance computers that are widely separated geographically. Anticipating top-quality performance for this supercomputer because of its innovative architecture, in 1999 we will write specifications for its multiteraops successor, called the SRC-7, if funded. In 2000, we will install an SRC-7 system in stages.

Such a powerful computing system will be needed at ORNL to help our scientists and engineers solve difficult Grand Challenge problems. Computer modeling on a teraops computer will lead to a more detailed understanding of the structure and mechanical behavior of metals and alloys. As a result of this information, these materials can be made stronger and more resistant to the effects of aging, radiation, and stress-corrosion cracking. Modeling may also be used to study an alloy's magnetic properties that affect its behavior.

Faster computer models are needed to tease out the details of combustion in spark-ignited and diesel engines. The information could speed the development of lean-burn natural gas vehicles that will use less fuel, reduce U.S. dependence on foreign oil, and produce lower carbon dioxide emissions, slowing the buildup of greenhouse gases in the atmosphere. The effects on future climate of increasing atmospheric concentrations of greenhouse gases requires complex simulations that teraops computing could make possible. Advances have been made in modeling the oceans and the atmosphere to pin down sources and sinks for greenhouse gases, but the influences of polar ice and land masses on future climate have not yet been factored in. Accurate models of the effects of pollution and greenhouse gases on future climate are needed to guide wise decisions by technical and political leaders.

How the chemical bases of long DNA strands containing genes are arranged, how genes produce proteins, how strings of amino acids fold into proteins, and how enzymes interact with protein receptors and with nucleic acids (DNA and RNA) are not well understood. Because of the huge amount of data from experimental approaches to these questions, sophisticated computational analysis is needed to make sense of this information. The more data there are, the more teraops computing will be needed to solve problems such as locating a particular gene and determining its structure and function, finding the set of genes that cause a fatal disease or unhealthful condition such as obesity, and designing a new drug.

Predicting the properties of plastics directly from their atomic structure has long been an elusive goal of polymer science, and it will continue to be. But calculations at the teraops rate will enable ORNL and University of Tennessee researchers to bridge from the results of atomistic calculations to those of calculations using approximate models that simulate polymer properties. The U.S. chemical industry has identified advanced computational modeling as a key technology that will enable molecular design of new plastics and other lighter, stronger materials of the future.

What features will enable the SRC supercomputers to perform more calculations at once and produce solutions faster than our Intel Paragons? For one thing, the central processing unit (CPU) chips that do computations will be much faster simply because they will be newer (remember Moore's law?). The Intel Paragons have Intel's older i860 chips, which aren't nearly as fast as the Pentium Pro chips in SNL's Intel Teraops computer. The SRC-7 machine will use the fastest CPU chips ever designed by Intel—the not-yet-released Intel Merced chips.

A second key improvement will be in the handling of computer memory. The multigigaops Intel Paragons in CCS have distributed memory—that is, each CPU has its own share of the total system memory. In this arrangement, any CPU that requires information stored in the memory of another must send a message requesting this information, which is then supplied by a response message through a sophisticated "message passing" system. The SRC supercomputers will have shared memory instead of distributed memory because all CPUs will be in direct contact with the entire machine memory. It will be easier for computer scientists to program a parallel machine with a shared memory than one with a message-passing distributed memory system. A shared memory will also allow faster retrieval of information.

A third feature will be the field programmable gate arrays (FPGAs). These FPGAs act as configurable special-purpose processors. They can execute multiple CPU instructions in one clock cycle. The reconfiguring of these FPGAs is easy, taking only 10 to 20 microseconds. They can be reprogrammed as often as desired.

SRC machines will have a fourth feature that will increase the speed of entering and retrieving information in a usable form (input-output, or I/O). SRC Computers, Inc., has placed an emphasis on the design of the I/O. By contrast, the Paragon XP/S 150 at ORNL has only one service processor for every eight computational processors. The improved processor ratio in the SRC machines should speed up I/O operations.

Evaluating Performance of the SRC-6

SRC machines are built from units called segments. Each segment is housed in a standard rack enclosure. Segments may be combined by linking the memory crossbar switches together to form larger shared-memory systems.

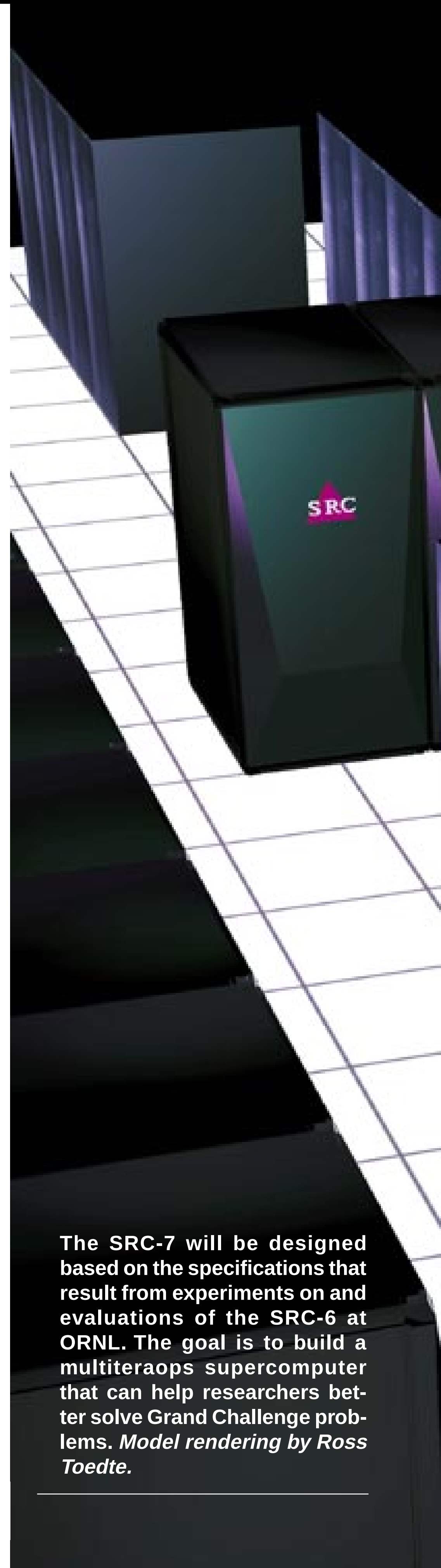
We will acquire two SRC-6 segments (see sketch on p. 20). We will evaluate their components and systems to determine strategies and mechanisms for interconnecting multiprocessor units. We will assess the use of FPGAs in various communication systems as well as options for programming frequently used application algorithms into FPGAs. This development effort by the CCS will be coordinated with other ORNL divisions and SRC.

CCS will initially evaluate the segment to determine if CPU performance, memory bandwidth, and I/O performance are properly balanced. We will then connect two segments using SRC's memory crossbar to form a larger, shared-memory machine. We will evaluate the new configuration, looking for weaknesses in the architecture that would prevent the machine from being scaled up to SRC's stated objective. In addition to testing the hardware, we will also test the scalability and performance of the system software and the user development environment provided by SRC. We will port a variety of our computer codes from the Paragon environment to the SRC system to see how well it performs on real codes.

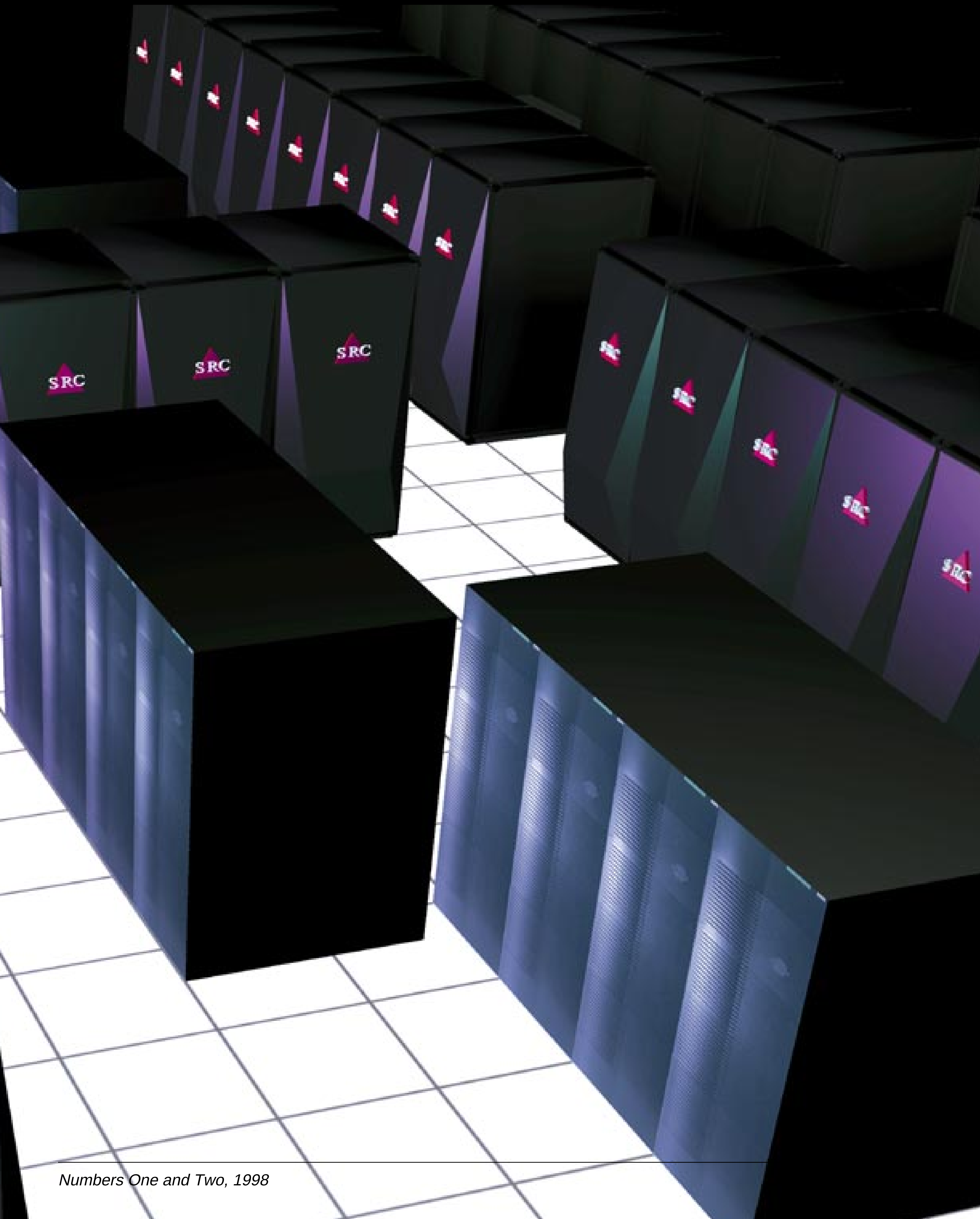
Once the performance of a single node is well understood, we will split the machine back into two segments and explore a variety of strategies for providing intermachine communications. We intend to work with SRC to develop several memory-connected communications channels to the SRC memory subsystem in a quest for highest performance. If our evaluation of SRC-6 verifies the excellence of its performance, as expected, we will write specifications and acceptance plans for an SRC-7 in FY 1999.

It should be emphasized that a shared-memory architecture provides a programming environment that hosts both shared-memory and message-passing applications. Shared-memory applications will port to the SRC system with a minimum of code changes. However, a major difference between shared- and distributed-memory architectures is that implementing a message-passing programming model on a shared-memory system is straightforward and efficient if sufficient memory bandwidth and capacity are present. However, implementing a shared-memory programming model on a distributed-memory system is not very efficient. Because the DOE energy research community has many codes developed for both types of parallel programming models, it is important that any large system support both types of programming model. Thus, it is essential that a shared-memory architecture with hundreds of processors (e.g., the planned SRC-7) has a memory subsystem with enough extra bandwidth to handle the message-passing traffic, as well as the memory requirements of the processors. In our evaluation of the SRC-6, we will determine the requirements for the SRC-7 in this area.

A multiteraops computer possessing a shared-memory architecture has long been a high-performance computing goal. A properly designed SRC-7 should meet that goal. We are focused now on the path to the SRC-7, which involves a detailed technical appraisal of the intriguing architecture incorporated in the SRC-6. This work is sponsored by DOE's Office of Energy Research, Office of Computational and Technology, Information, and Computational Sciences. The CCS-ORNL team that made the Intel Paragons hum is most pleased that the initial step on this path has been taken and looks forward to the technical challenges of the comprehensive evaluation of the SRC-6. The journey should help ORNL reclaim its position near the top of the high-performance computing hierarchy by the start of the next millenium.—Based on information provided by Ken Kliewer, director of the CCS, and Arthur S. (Buddy) Bland, also of the CCS



The SRC-7 will be designed based on the specifications that result from experiments on and evaluations of the SRC-6 at ORNL. The goal is to build a multiteraops supercomputer that can help researchers better solve Grand Challenge problems. *Model rendering by Ross Toedte.*


SRC

Biological Sciences

Learning the genetic causes of human diseases and finding better ways to prevent and cure diseases are long-term goals of ORNL's studies in the biological sciences. Our talented staff and excellent facilities for genetics research, information and computational biology, protein engineering, and structural biology not only help us attain these goals but also support extensive industrial and educational outreach programs.

At our Mouse Genetics Research Facility, where functional genomics research is performed, researchers have determined that the mutant mouse agouti gene has a primary, rather than an indirect, role in promoting skin cancer. Modern technologies are helping ORNL biologists assess hidden genetic defects (from depression to digestive disorders) in the descendants of irradiated mice. ORNL nuclear medicine experts have developed a technique that is expected to benefit heart patients. Clinical tests are being conducted on patients to determine if radiation from the rhenium-188 isotope produced by ORNL's generator prevents the reclogging of coronary arteries after the patients have balloon angioplasty operations. These achievements promise to advance our understanding of the origins of cancer, behavioral disorders, and heart disease and speed the development of ways to treat these health problems.

A normal mouse and an obese mouse that has the mutant agouti gene.

Agouti Gene Linked to Mouse Skin Cancer

ORNL researchers have determined that the mutant mouse agouti gene has a primary role in promoting skin cancer.

The normal, or wild-type, mouse (top) has agouti colored hairs, which are black with a central band of yellow. The mouse at left has completely black hair because it lacks the agouti gene. The mouse at the bottom is mostly black with some yellow hairs because it has a partially inactive agouti gene. The yellow mouse has an overactive agouti gene that is turned on all the time throughout the body. The overactive agouti gene also causes mice to become obese and diabetic and to develop cancer. *Electronic file of photograph by Tom Cerniglio enhanced by Allison Baldwin.*

Mice, squirrels, and other mammals often have brown fur streaked with gray. The alternating light and dark bands of fur that make mice look grizzled result from the action of the agouti gene (named for the South American rodent). This mouse gene, whose normal and mutant forms were identified and cloned by Ed Michaud and others at ORNL in 1992, is of interest to researchers. The reasons: its mutant form is linked to altered fur color, obesity, diabetes, and cancer in mice, and it has a human counterpart.

When the mouse agouti gene is functioning normally, it turns on briefly in the skin where hair follicles are rooted. There, ORNL researchers found, the gene causes the secretion of the agouti protein, which signals the pigment-producing melanocyte cells to make yellow instead of black pigment for awhile. Then when the agouti gene turns off, the melanocyte cells return to producing black pigment again. Thus, a normal mouse hair is black at both ends, with a band of yellow in between.

But what happens if this coat color gene is mutated or deleted? Michaud and other ORNL researchers found that the mutant agouti gene expresses itself all the time, causing the melanocyte cells to produce yellow pigment endlessly. Thus, mutant agouti mice are yellow. And if a mouse is born without an agouti gene, its coat color will be solid black.

Being yellow is the least of the mutant agouti mouse's problems. It also is obese, diabetic, and more susceptible to getting skin, lung, liver, and mammary gland cancer. An explanation for these widespread disease effects may lie in the ORNL discovery that the mutant agouti gene's single defect is that it codes for the production of normal agouti protein not only all the time but also in every mouse cell. The causes for this ubiquitous, unending expression appear to be additions of DNA not usually found within the gene, such as retroviruses and a promoter usually linked to the nearby Raly gene, which is mostly deleted as part of the agouti gene mutation.

ORNL researchers and collaborators have found that the melanocyte receptor to which a ligand binds to activate the cell's black pigment production is blocked by signals from the agouti protein, resulting in yellow pigment production. It has also been discovered that four receptors in other parts of the body have similar structure and function, suggesting that the receptors' normal activity in regulating body processes may be susceptible to disruption by the agouti protein.

In a long-term quest to identify the mechanisms underlying obesity, diabetes, and cancer in yellow mice, ORNL researchers set out first to prove that overproduction of the normal agouti protein by an overactive gene causes these diseases. To address this point, they made transgenic mice by inserting into fertilized mouse eggs the normal agouti gene linked to a special beta-actin promoter, a DNA fragment that causes the gene to be turned on all the time everywhere in the body. The transgenic mice were born with yellow hair and became obese and diabetic, demonstrating that overproduction of the normal agouti protein causes these diseases.

In a recent set of experiments, Michaud and his colleagues next asked if the mouse agouti gene has a primary role in promoting skin cancer or if the cancer is a secondary effect of obesity and diabetes (e.g., from excessive levels of insulin produced to clear glucose from the blood). To tease out this information, they used different transgenic mice that had an active agouti gene only in the skin. In this case, the normal agouti gene was linked to a keratin promoter that causes genes to be turned on only in skin. These transgenic mice have yellow hair but are not obese or diabetic. In experiments involving large numbers of transgenic and control mice (black mice with no active agouti gene), ORNL researchers found that only 3% of the control mice developed skin cancer but 20% of the transgenic mice got the disease. Thus, ORNL demonstrated that overproduction of the agouti protein by the overactive agouti gene has a direct role in causing skin cancer.

Funding for the research came from DOE's Office of Biological and Environmental Research.

Observing Subtle Changes in Mutant Mice

Modern technologies help ORNL biologists assess subtle genetic defects in the descendents of mice exposed to radiation and chemicals.

Dabney Johnson watches a mutant mouse afflicted with "behavioral despair" (left) make no effort to escape the water in a tank while the normal mouse swims rapidly in an effort to get out of the water during the Porsolt swim test. *Photograph by Tom Cerniglio.*

Shortly after World War II, geneticists Bill and Lee Russell established a mammalian genetics program at ORNL to assess the genetic effects of ionizing radiation and a wide variety of chemicals in mammals. Many mutations that cause visible changes in the color or form of the mouse were generated, as were genetic changes that cause embryos to fail to develop or mice to die after birth. In some cases, the DNA damage that caused these visible or lethal mutations also caused more subtle genetic changes that would not traditionally have been recognized. To evaluate mutants for behavioral and biochemical changes, ORNL researchers are developing new technologies and increasing the sophistication, efficiency, and throughput for these tests.

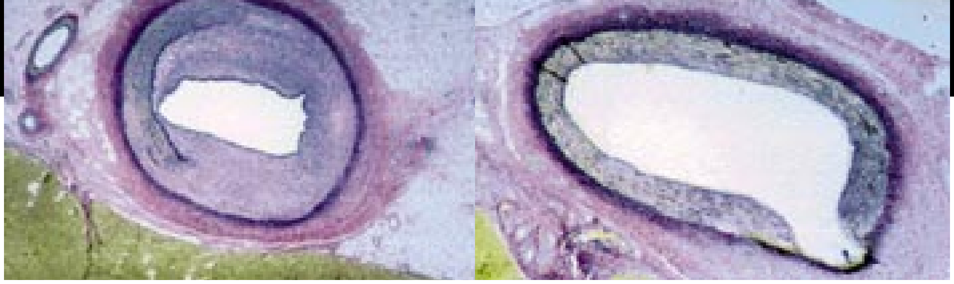
Using recombinant DNA techniques to identify and characterize genes from two small regions of chromosome 7 near the pink-eyed dilution (*p*) gene, ORNL researchers have identified less obvious defects in mice caused by the absence of certain genes in the *p* neighborhood. These defects include memory loss and depression.

Noticing that some of the genes in the *p* neighborhood are involved in regulating the activity of cells in the central nervous system, ORNL researchers led by Dabney Johnson recently gave strains of mice missing these genes two behavioral tests. The first examines the mouse's ability to process and store new information—that is, to remember an unpleasant experience. This test consists of a gentle foot shock accompanied by a sound cue; the mouse is then retested without the shock to see if it is afraid of both the sound that accompanied the shock and the chamber in which the shock took place. Normal mice fear both the sound and the chamber, while mice with the mutation near *p* fail to remember that the sound and chamber are associated with an unpleasant experience. ORNL researchers are focusing on this small region of the mouse genome to identify this gene, and eventually its entire associated biochemical pathway, which affects learning and memory.

The second test is the Porsolt swim test for behavioral despair, the equivalent in mice of human depression. Mice are put into a water tank from which they cannot escape. During the 7-minute test, a normal mouse will try constantly to climb out, but mice with the mutation near *p* exhibit despair and make little effort to escape.

Biochemical tests have shown that a particular region of the brain in these mutant mice has low levels of serotonin, a neutrotransmitter that promotes communication among brain cells called neurons. Low levels of serotonin have been associated with depression in people. Because the antidepressant drug Prozac raises the level of serotonin in humans, the ORNL biologists will give Prozac to the defective mice to see if it improves their performance in the Porsolt swim test. The research could lead to a more-targeted, lower-dose treatment that raises the serotonin level only in a specific part of the brain, rather than in the whole body, to dispel behavioral despair.

The funding for this research came from DOE's Office of Biological and Environmental Research.



Inhibition of restenosis (artery reclogging) using rhenium-188 was demonstrated in a swine coronary balloon overstretch injury model. Left: Control artery 30 days after balloon overstretch injury. Right: injured artery 30 days following rhenium-188 irradiation. *Images courtesy of Judah Weinberger.*

ORNL Isotope Offers Hope for Heart Patients

Radiation from the rhenium-188 isotope produced by ORNL's generator may prevent the buildup of smooth muscle cells (restenosis) in coronary arteries after balloon angioplasty.

Harry and Matilda are among the unlucky 30%. Both had mild heart attacks because a coronary artery had been narrowed by the accumulation of fatty deposits. Both had a procedure called coronary angioplasty to restore full blood flow to the heart muscle. In this procedure, a catheter equipped with a tiny uninflated balloon at the tip is inserted into a femoral artery in the leg and then threaded through the clogged coronary artery. Then the balloon is inflated to clear the blockage and widen the artery. But six months later, as happens with at least 30% of the 450,000 Americans who have the angioplasty procedure each year, Harry's and Matilda's treated arteries developed a different type of blockage. They were reclogged by the buildup of smooth muscle cells in response to balloon-induced vessel damage, a condition known as restenosis.

Most people in the unlucky 30% undergo additional angioplasty or heart bypass surgery to unclog their reclogged arteries. Nationally, these necessary second operations add $1 billion to the $4 billion cost per year of the initial angioplasty procedures. Fortunately, a promising cure for restenosis is radiation.

Although many radioisotopes and delivery systems are being evaluated for this purpose, a tungsten-188/rhenium-188 generator system developed at ORNL for cancer therapy has distinct advantages. This cylindrical system uses the radioisotope tungsten-188 from ORNL's High Flux Isotope Reactor. At the top of the cylinder, tungsten-188 binds tightly to aluminum oxide powder saturated with acidic saline. As it decays, the tungsten turns to rhenium-188, which lets go of the powder. A solution of rhenium-188 is obtained by washing the radioisotope down from the top.

Using a tiny iridium-192 wire source threaded through the coronary artery, cardiology researchers at Columbia University had demonstrated in pigs that high radiation doses inhibit muscle cell proliferation in newly unclogged arteries. Because of difficulty in centering the wire, the radiation dose was not being uniformly delivered to the damaged arterial wall.

Arnold Beets and Russ Knapp show a mockup of a tungsten-188/rhenium-188 generator system for use in preventing a heart patient's coronary arteries from reclogging after balloon angioplasty. *Photograph by Jim Richmond.*

To deliver a more uniform dose, Judah Weinberger, a Columbia University cardiologist, conceived of using a radioisotope solution to inflate the balloon at low pressure following high-pressure balloon inflation with saline to unclog the artery. Searching for the radioisotope with the best properties for this application, he called ORNL's Russ Knapp, who proposed rhenium-188 because ORNL's generator system can produce hundreds of doses of rhenium-188 in solution over several months in a hospital. Rhenium-188 also has nearly perfect beta particle energy for optimal vessel irradiation. Also, because rhenium would be rapidly excreted from the bladder in the unlikely event of balloon rupture, it is safe for patients and should receive regulatory approval.

ORNL is providing Columbia University with the radioisotope generator. ORNL researchers also developed a simple, efficient method for concentrating the rhenium-188 solution obtained from the generator because of the small volume of the balloons and the high radiation levels of rhenium-188 required for the short irradiation times. The patented ORNL method provides a high enough concentration of rhenium-188 to deliver the proper dose. Exclusive rights to this method were licensed in July 1997 to Mallinckrodt Medical, Inc., an international radiopharmaceutical manufacturer headquartered in St. Louis.

Use of rhenium-188 for human patients in clinical trials at Columbia University Medical Center in New York City was approved by the Food and Drug Administration. By March 1998, several patients had been treated with the rhenium-188 angioplasty procedure. Similar clinical studies are being carried out at the Royal Perth Hospital in Perth, Australia, and in the departments of nuclear medicine at the universities of Dresden and Ulm in Germany.

This partnership involving private business and university and government researchers is expected to benefit many thousands of people and improve their quality of life. If Harry's and Matilda's need for angioplasty had arisen a few years later, they might have been among the luckier patients.

The project was funded by DOE's Office of Biological and Environmental Research.

Environmental Sciences and Technology

Energy development, production, and use can induce major environmental and health problems, such as fish kills and respiratory disease. To better understand these problems and develop solutions in response to DOE's concerns, ORNL takes an interdisciplinary approach by integrating a broad spectrum of disciplinary foundations (biology, chemistry, computational sciences, ecology, engineering, geology, geochemistry, geophysics, hydrology, physics, toxicology, and social sciences). Our work, which is anchored in a strong fundamental research program, extends to applications in human health, biotechnology, environmental protection and remediation, separations science, and studies of global change and sustainable development. Facilities for biotechnology, bioprocessing, and ecological and environmental studies support extensive industrial and educational outreach programs.

In 1997, ORNL played a major role in DOE's 11-lab report on technology opportunities to cut greenhouse gas emissions. ORNL researchers have been using computer modeling to better understand how terrestrial ecosystems influence carbon dioxide concentrations in the atmosphere; they found that, in a growing season during an El Niño Southern Oscillation, terrestrial ecosystems take up 1 to 2 billion tonnes of additional carbon. ORNL researchers have been applying scientific knowledge to help Guatemala address its biodiversity and environmental problems and to raise the standard of living of rain forest residents. ORNL has discovered ways to orient electrically charged spinach leaf proteins, bringing us closer to biomolecular electronic devices based on spinach, not silicon. In environmental technology, we are mapping the effectiveness of bacteria in breaking down chlorinated solvents contaminating soil at an Air Force base.

Strengthening Environmental Management in Guatemala

ORNL is helping Guatemala improve its environmental management and decision-making to protect its biodiversity.

In the Peten region in northern Guatemala lies an enormous rain forest. It is a treasurehouse of biodiversity and the largest carbon sink in the Western Hemisphere north of the Amazon River. Because of Guatemalans' demands for jobs, homes, and farm land, this region has been threatened by deforestation, which can eliminate endangered species of medicinal value and increase global greenhouse gas concentrations. By the late 1980s, it was feared that the region would be completely deforested within three decades if nothing was done.

As a part of its development assistance programs in Guatemala, the U.S. Agency for International Development (USAID) established a Mayan Biosphere Project (MBP) in 1991. The goals were to help preserve the rain forest and raise the standard of living for the region's people, many of whose Mayan ancestors go back 1000 years. USAID asked ORNL to organize and lead the multiyear project through an interagency agreement with DOE. The project involved working with a diverse team of nongovernmental environmental organizations and local groups.

ORNL's Keith Kline was assigned to live in Guatemala City, where he has served as the USAID Mission's environmental officer and leader of the project, with support from other ORNL staff members. Since MBP began operating in 1992, the project has significantly slowed the rate of deforestation in the Peten region and helped its 400,000 residents shift to a lifestyle less destructive of the forest. For example, instead of clearing forests to grow corn and beans, some people collect and sell forest products. Others have improved cultivation practices and introduced agroforestry. As a focus for the effort, the project established a national park to provide effective environmental management in the area.

In 1996, a formal evaluation of all USAID environmental programs worldwide ranked MBP number one in effectiveness. In 1997 the agency's Latin American and Caribbean Bureau ranked it first in performance in the hemisphere. In 1996, USAID extended MBP for four additional years through March 2000, with a total estimated life-of-project budget of $50 million.

One aspect of the extension added a new policy component intended to improve the capacities of Guatemalan government agencies (equivalents of the U.S. EPA and National Parks Service) to manage the environment for the long term. Since then, ORNL's Tom Wilbanks, Tim Ensminger, Bob Perlack, and Sherry Wright have traveled frequently to Guatemala to meet two challenges: assisting Guatemalan partner agencies in conducting environmental impact and policy assessments related to the most pressing national controversies and setting up a partnership between ORNL and a Guatemalan counterpart, Fundación Solar, to transfer expertise.

The first of the controversies was provoked by a proposal from a U.S.-based multinational forest products firm. It sought to transport logs from a Guatemalan tree plantation to the Atlantic coast by barge on the scenic Rio Dulce, through the heart of a national park, and to construct a barge terminal at the park's edge. This proposal was heatedly opposed by environmental groups and advocates of ecotourism development. USAID asked ORNL to assist Guatemala's equivalent of the EPA in assessing the environmental impacts of the proposed activity and suggesting alternatives to the proposed action. ORNL's work became not only a basis for discussions at the highest levels of government but also has been widely recognized as setting a new standard for improving information for environmental decision making in Guatemala. In the end, the Guatemalan president disapproved the proposal, but discussions continue on other alternatives, influenced by ORNL's analysis.

As a part of this assessment, ORNL recommended that the country develop a workable environmental management plan for the Rio Dulce area. In 1997 the Laboratory was asked to help organize and lead an effort to develop such a plan, which would give Guatamalans their first experience with a public participation process.

What makes ORNL's accomplishments different from those of, say, a consulting firm is that our assistance is grounded in knowledge obtained through our research in environmental management, environmental impact assessment, biodiversity protection, global climate change, and energy and environmental institution building. Besides applying this knowledge to foster sustainable development, we are bringing back from Guatemala unanswered research questions that may be added to future research agendas.

The project was funded by USAID through an interagency agreement with DOE.

Tim Ensminger (second from right) is one of several ORNL researchers who assessed the environmental impact of a proposed log barging operation on the Rio Dulce (river shown behind the men on the boat dock and in the photograph on opposite page) as a part of an environmental assessment of the Rio Dulce National Park in Guatemala.

ORNL's Big Role in a Major DOE Study

ORNL played a major role in DOE's 11-lab report on technology opportunities to cut greenhouse gas emissions.

In an address to the United Nations in June 1997, on the occasion of the fifth anniversary of the Rio Conference on the Environment, President Clinton spoke on the need for a vigorous technology research, development, and demonstration (RD&D) program to address the challenge of global warming. He noted that the United States has only 4% of the world's population yet produces more than 20% of its greenhouse gases, largely because the nation relies primarily on fossil fuels to heat, cool, and light buildings, run its factories, and power its vehicles. "In order to reduce greenhouse gases and grow the economy," he said, "we must invest more in the technologies of the future. Government, universities, business, and labor must work together. All these efforts must be sustained over years, indeed decades."

Following this address, President Clinton directed his cabinet to respond to the challenge of reducing greenhouse emissions in the United States. In turn, Energy Secretary of Energy Federico Peña asked ORNL Director Alvin Trivelpiece and Richard Truly, director of the National Renewable Energy Laboratory, to lead a DOE national laboratory effort to identify cost-effective technologies to reduce greenhouse gas emissions. A team of 11 laboratories was mobilized to respond to this request. The result was a two-volume report entitled Technology Opportunities to Reduce U.S. Greenhouse Gas Emissions.

More than 150 persons from all 11 national laboratories participated in the effort, and at times as many as 300 people across the DOE system were involved. Because of the need to complete the report on a compressed schedule, the report was planned, written, and revised largely through electronic mail submissions, conference telephone calls, and reviews of draft reports that were posted on the World Wide Web. At ORNL some 30 scientists, managers, writers, editors, artists, and electronic publishers were involved in putting together the report.

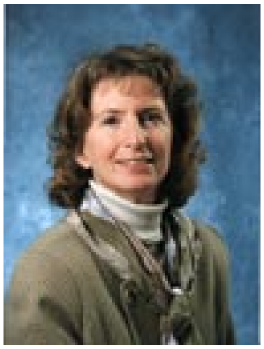
The report describes technology opportunities "that have significant potential to reduce greenhouse gas emissions" between now and 2030. In its second volume, 47 specific technology pathways are profiled. These technologies fall in three categories: energy efficiency, clean energy, and carbon sequestration (removing carbon from emissions and increasing storage of carbon). DOE is already developing many energy efficiency technologies, such as refrigerators and cars that will be two to three times more efficient than today's models. The report proposes a strategy to improve and increase the use of clean-energy sources that emit little or no carbon, such as natural gas burners, nuclear power plants, renewable energy (e.g., solar and wind power, electricity and fuels from agricultural biomass), and fuel cells that use hydrogen to produce electricity. Carbon emissions could also be reduced by switching transportation fuels from gasoline to biodiesel fuel and ethanol; by distributing electricity more efficiently using superconducting transformers, cables, and wires; and by removing carbon from fuels before combustion. The third category of technology pathways includes those that would efficiently remove carbon dioxide from combustion emissions before they reach the atmosphere or would increase the rate at which oceans, forests, and soils naturally absorb atmospheric carbon dioxide. Technologies to store carbon deep in the ground or in aquifers over a long time might also be devised.

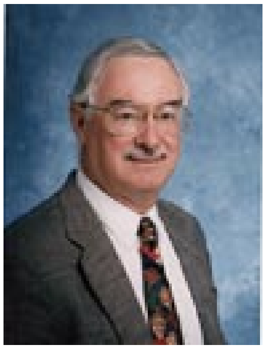
In the report, the DOE lab directors conclude that (1) by 2030, a vigorous RD&D program could deliver a wide array of cost-effective technologies that together could reduce the nation's carbon emissions by 400 to 800 million tonnes of carbon per year; (2) basic research is needed to advance science and technology enough to reduce U.S. greenhouse gas emissions significantly yet sustain economic growth, partly through side benefits such as improved air quality, reduced U.S. dependence on imported oil, and increased exports of U.S. technologies to help other nations reduce their greenhouse gas emissions; (3) adequate support for an accelerated RD&D program could be double the current levels of funding for development of energy-efficiency technologies; and (4) strategic public-private alliances provide the best approach for developing and deploying most greenhouse gas-reduction technologies.

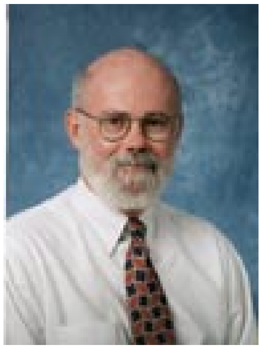
The report recommends that the United States develop and pursue a detailed, comprehensive technology strategy for reducing greenhouse gas emissions. Implementing such a strategy, the report states, would be an "investment insurance policy," one that "DOE's national laboratories stand ready to champion."

Other DOE national laboratories that contributed to the report were Argonne, Brookhaven, Idaho (INEEL), Lawrence Berkeley, Lawrence Livermore, Los Alamos, Pacific Northwest, Sandia, and the Federal Energy Technology Center.

David Reichle, Marilyn Brown, John Sheffield, and Mike Farrell were the technical co-leaders for the planning and drafting of the DOE report, which was released by Secretary Peña on Earth Day, April 24, 1998 (see http://www.ornl.gov/climate_change).







Why Carbon Storage on Land Varies

ORNL researchers are using computer modeling to better understand the influences of terrestrial ecosystems and climatic variation on atmospheric CO_2 content.

What goes up sometimes comes down. By burning gasoline to power cars and trucks, coal to produce electrical power, and forests to clear land for agriculture, people have altered the earth's atmosphere. Fossil fuel combustion and forest clearing currently inject 8 billion tonnes of carbon per year into the atmosphere, which, combined with the carbon dioxide (CO_2) already naturally present, could speed the onset of global warming.

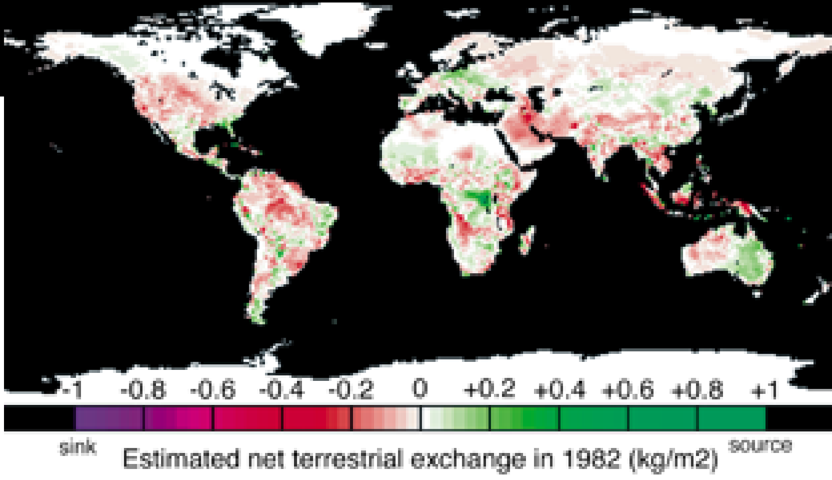
The good news is that not all the carbon added each year stays in the atmosphere. According to computer model estimates, about one-third of this amount is later taken up by the oceans. Another one-sixth (1.5 to 2 billion tonnes) is removed from the atmosphere at least temporarily by the world's terrestrial ecosystems—forests, vegetation, soils, farm crops, and pastures. But terrestrial ecosystems are a source of carbon to the atmosphere as well as a sink for its carbon. Although 15% of all atmospheric carbon, or about 120 billion tonnes, is annually taken up by trees and vegetation for photosynthesis to build plant tissue, about an equal amount is returned to the atmosphere as carbon dioxide from both plant respiration and the decomposition (by bacteria and fungi) of plant litter and soil organic matter. Another small source of carbon from terrestrial ecosystems is forest fires.

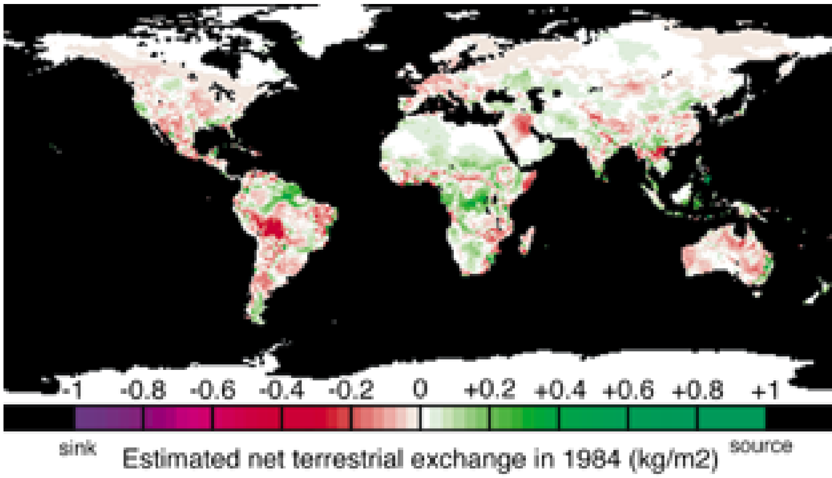
Scientists are unable to determine where 0.5 to 1 billion tonnes of carbon goes each year after it enters the atmosphere. They are trying to account for the "missing" sink required to balance this century's global carbon budget. How much of this carbon goes to the ocean and how much is absorbed by terrestrial ecosystems? It is not now possible to directly observe exchanges between the atmosphere and terrestrial systems at regional, national, or global scales because of the large magnitudes and temporal variations of natural carbon cycle fluxes and the vast amount of carbon stored in vegetation and soil.

What is the fate of the unaccounted-for carbon? To help find out, ORNL researchers led by Wilfred (Mac) Post are using computer modeling to better understand how terrestrial ecosystems influence CO_2 concentrations in the atmosphere. They have discovered that, in the past 100 years, environmental conditions have changed slightly, enabling plant biomass to increase and terrestrial ecosystems to soak up more CO_2. Plants may be growing faster and larger because they are being "fertilized" by increased atmospheric concentrations of CO_2 and increased deposition of air pollutants containing nitrogen, a plant nutrient. Even more significant, the ORNL computer model results show that carbon exchanges between the atmosphere and terrestrial ecosystems are sensitive to climate variations, such as the increase in average global temperature of 0.5°C (1°F) over the past 100 years and the El Niño-Southern Oscillation, the large-scale climatic fluctuation of the tropical Pacific Ocean marked by a warm surface current. In a growing season during an El Niño, terrestrial ecosystems take up 1 to 2 billion tonnes of additional carbon, but much of that extra biomass may decompose and release carbon in succeeding years.

When climate change alone is considered, according to model results, carbon storage in the global terrestrial biosphere decreased by 1% from 1900 through 1988. However, when a moderate CO_2 fertilization response was added in the model, terrestrial carbon storage increased by 3% because plants took up more carbon for photosynthesis than they released through respiration. In short, terrestrial ecosystems have become more of a carbon sink than a source over the past 100 years. Also, computer model results suggest that climate change combined with CO_2 fertilization increased carbon storage in terrestrial ecosystems enough to account for 55 to 70% of the missing sink from 1900 through 1988.

ORNL's models indicate very large year-to-year variations in net carbon exchange between terrestrial systems and the atmosphere—on the order of 1 to 3 billion tonnes in either direction. Whether the larger fraction of carbon goes up or down in atmosphere–land exchanges depends on large-scale climate fluctuations.





The estimated net ecosystem production (plant biomass growth) changed by 2 billion tonnes of carbon globally between 1982 and 1984 as a result of changing weather patterns produced by the 1982–83 El Niño.

The research was sponsored by DOE's Office of Biological and Environmental Research, Environmental Sciences Division, Carbon Dioxide Research Program.

Spinach Power: Biomolecular Electronics

ORNL has discovered ways to orient electrically charged spinach leaf proteins, bringing us closer to biomolecular electronic devices.

The next generation of optoelectronic devices may be based on spinach, not silicon. Photosynthetic reaction centers from spinach could be used for super-high-resolution video imaging, ultrafast switching, and solar power generation.

Green plant leaves contain two pigment protein complexes that convert light energy into chemical energy (photosynthesis). Both chlorophyll-containing proteins—called Photosystem I (PSI) and Photosystem II (PSII)—use the energy of the sun to make plant tissue. When each of these photosynthetic reaction centers receives a photon of light, charge separation can occur in 10 to 30 picoseconds—100 times faster than a silicon photodiode. If these photosynthetic reaction centers could be lined up perpendicular to a metal surface, current would flow, and biomolecular electronic devices would be possible.

In the past decade, ORNL researchers Eli Greenbaum, James Lee, and Ida Lee came up with a number of significant ideas and findings. First, PSI and PSII can be isolated from spinach leaves. Second, PSI and PSII can be rewired to produce fuels by metallocatalysis and photosynthetic water splitting ($2H_2O = O_2 + 4H^+ + 4e^-$). In plants, the photoenergized electrons are used to form carbohydrates (CH_2O) to build plant tissue. But these electrons ($2e^-$) can also be made to recombine with the protons ($2H^+$) to yield hydrogen by metallocatalysis, or the electrons can be put to work as electric current. The group demonstrated that spinach PSI and PSII together can be made to produce both oxygen and hydrogen, a clean fuel.

To generate electrical current, the researchers found they had to provide PSI reaction centers with an electrical contact and a preferred orientation. They learned how to deposit platinum (a good electrical conductor) on one end of PSI. They showed that platinum anchors PSI to a gold surface and that it does not damage PSI or render it inactive.

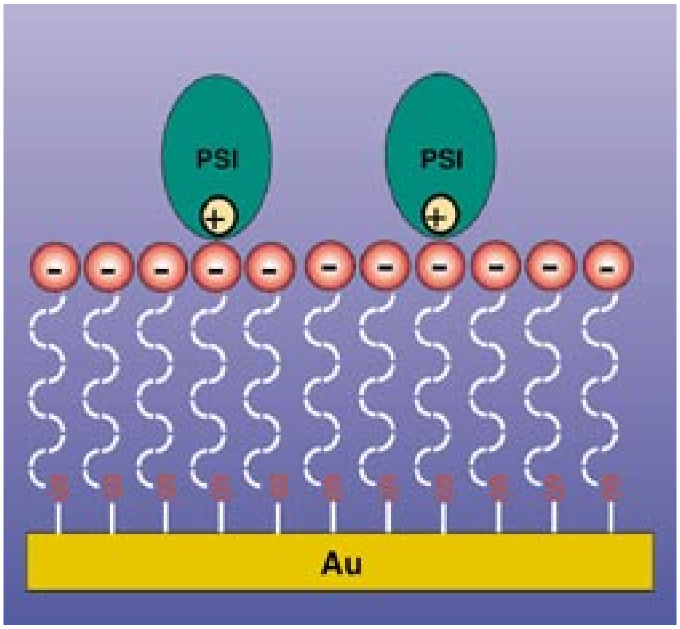
The next hurdle was to orient the PSIs so that the same ends point in the same direction. A scanning tunneling microscope (STM) was used to determine the orientation of each PSI because the tunneling current is affected by the preferential direction of the electron flow. PSI will act like a current rectifier under the STM if it is perpendicular to the surface. If a PSI is parallel to the surface, it will act like a semiconductor instead. If all PSIs are perpendicular to the surface, current will flow only if all are pointing in the same direction, but not if half are pointing up and half down.

The initial success at turning a PSI molecule at will came when the group deposited a nanometer layer of platinum atoms on the reducing end of a PSI, which is positively charged. The deposited platinum weakened the electrostatic attraction of that end for a negatively charged gold surface, causing the other positively charged end to be more strongly pulled to the gold surface.

In 1997 the ORNL group found an even better way to achieve preferred orientation of PSIs: chemical treatment of the atomically flat gold surface on a mica substrate. They coated gold surfaces chemically with three different chemicals and reported the results in the October 27, 1997, issue of *Physical Review Letters*. No preferential orientation was observed with 2-dimethylaminoethanethiol. "For mercaptoacetic acid," they reported, "83% of the PSI reaction centers were parallel to the surface, whereas for 2-mercaptoethanol, 70% were oriented perpendicularly in the 'up' position and only 2% were in the 'down' position." Apparently, the sulfur atom in each molecule binds strongly to gold, and the other end selectively binds to the oppositely charged part of a PSI, causing it to point either up, down, or parallel to the surface. Thus, PSI reaction centers can be selectively oriented by chemical modification of a gold surface.

These findings suggest the feasibility of the concept of a "lean clean green machine" that uses sunlight and operates without fossil fuels. Such a machine could meet many DOE mission goals by generating electrical power, producing clean hydrogen fuel, and fixing carbon dioxide on a ruthenium film to produce methane fuel, reducing the atmospheric content of greenhouse gases. It could be a DOE dream machine.

The research was supported by DOE's Office of Computational and Technology Research, Advanced Energy Projects and Technology Research Division, and DOE's Office of Basic Energy Sciences, Division of Chemical Sciences.



Electrically charged platinized Photosystem I (PSI) reaction centers from spinach leaves are oriented in the same direction, making possible the development of biomolecular electronic devices. The gold (Au) base is treated with a chemical whose sulfur (S) atoms bind strongly to gold. The negatively charged ends of molecules in this chemical selectively bind to the positively charged free ends of the PSIs. As a result, all PSIs point in the same direction. *Drawing by Ida Lee.*

Intrinsic Bioremediation Across a Plume of Chlorinated Solvents

ORNL researchers are helping define a method for determining whether bacteria at a given site will effectively degrade contaminants such as trichloroethylene.

A member of the project team cuts a sediment core using sonic drilling at Dover Air Force Base. ***Photograph by Susan M. Pfiffner.***

Chorinated solvents, including trichloroethylene (TCE), are the most common contaminants in soil and groundwater because they are used as solvents and degreasers in manufacturing, maintenance, and service installations. Elimination or treatment of such contaminants through methods such as pump-and-treat technology and soil removal can be difficult and expensive. Fortunately, soil and groundwater contaminated with TCE often contain bacteria that break it down. In fact, under certain conditions, chlorinated solvents are completely degraded naturally to harmless end products through microbial action, a process known as intrinsic bioremediation. ORNL researchers are participating in a study at Dover Air Force Base (AFB) to help define a method for determining whether in situ biological destruction will occur at a given site. If the conditions for intrinsic bioremediation are present, expensive measures can be avoided.

Bioremediation is possible if the kinds of microorganisms that will destroy the contaminant are already present and if they exist in adequate numbers across the contaminated area, or contaminant plume. In the case of TCE, these organisms are not likely to be present unless contaminants other than TCE are present because the bacteria prefer to feed on the other contaminants. So bioremediation is a very likely possibility if TCE is a contaminant in a landfill or a swamp, and not likely if TCE is simply found in a clean sand environment. In the case of Dover AFB, gasoline is also present as a contaminant, so it was thought that bacteria that feed on gasoline would be present in adequate numbers to break down most TCE there.

The problem in likely bioremediation sites is to determine whether in situ biological destruction is proceeding at a rate that will degrade the contamination effectively—and uniformly in all directions. To date, little evidence has been obtained regarding the changes in microbial population and activity, or heterogeneity, across subsurface and flowing-sand aquifers. Recent analyses by the ORNL investigators have demonstrated significant differences in rock strata, microbial biomass, and microbial diversity in both the horizontal and vertical directions. Typically, their geostatistical analysis has revealed significant heterogeneity at scales of greater than 1 meter. At these scales, the heterogeneity of the microbial populations is apparently closely tied to the geochemical and physical environment. These changes can be pronounced across regions with differing physical and geochemical properties.

In order to study horizontal subsurface heterogeneity across the TCE plume at the Dover AFB test site, researchers used sonic drilling technologies, proven at uncontaminated sites, in a TCE-contaminated aquifer. Sampling in sand aquifers with ordinary drilling methods is unsatisfactory because sand very rapidly seeps into the sampling area, and it is consequently impossible to define the exact location of the sample. In "sonic drilling," a rapidly vibrating drill is inserted into the aquifer. This technique obviates the problems of ordinary methods and allows the researcher to determine exactly the location of the sample. The sampling consists of multiple drillings across a horizontal cross section of the aquifer. The drilling equipment, which is supplied by a subcontractor, can be set up in only a few minutes and takes 10- to 20-ft cores at depths of 50 to 60 ft. The results of these studies will expand the understanding of the heterogeneity of microbial activity and community structure in the subsurface and its impact on the bioremediation process.

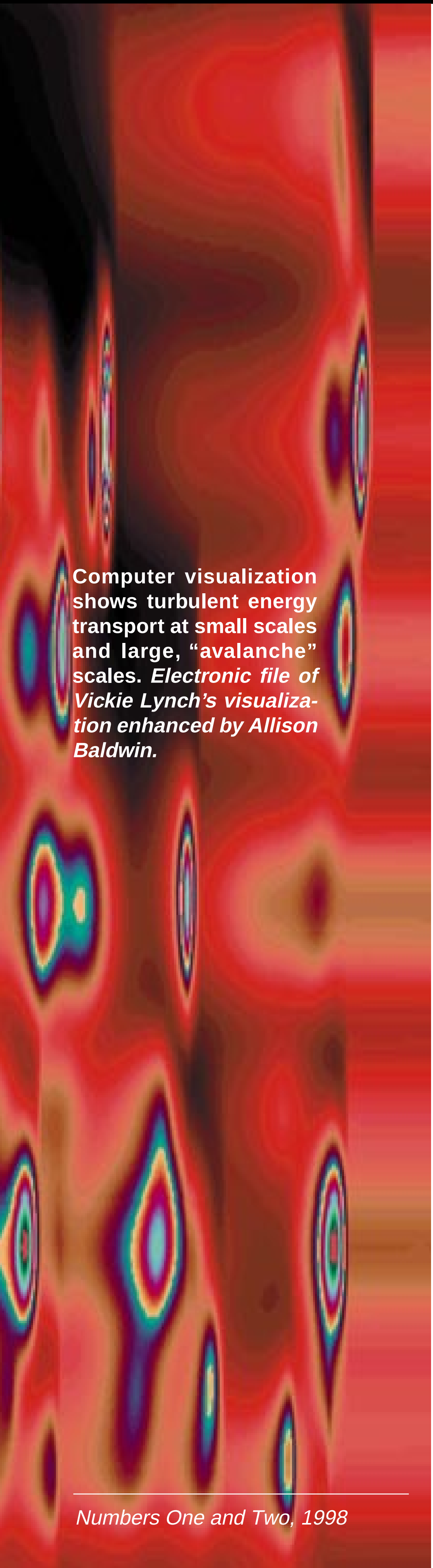
The work is sponsored by the U.S. Department of Energy, the U.S. Department of Defense, the U.S. Environmental Protection Agency, and industry, through the Remedial Technology Development Forum.

Energy Production and End-use Technologies

Clean, efficient, safe production and use of energy have long been goals of ORNL research and development. At first our focus was fission energy. Then we started research efforts in fusion, fossil, and renewable energy as well as energy efficiency. Among our achievements in 1997 were collaborations with industrial organizations to develop a high-temperature superconducting cable for underground power transmission and a high-temperature superconducting transformer for industry. In the area of transportation, we helped determine the effectiveness of novel catalysts in reducing nitrogen emissions from highly efficient diesel cars of the future. In fusion energy research, we found success and gained recognition at the White House for using the model of a sandpile to better understand and control fusion plasma turbulence and energy losses.

ORNL is one of the world's premier centers for R&D on energy production, distribution, and use and on the effects of energy technologies and decisions on society. As a primary performer of DOE-sponsored R&D in energy efficiency, ORNL applies distinguishing capabilities in materials science, biotechnology, engineering, and technology development and evaluation to transportation systems, biofuels, efficient buildings and building materials, industrial processes, and utilities.

ORNL research on energy technologies applies the Laboratory's strengths in physics and engineering to the improvement of existing systems and the development of new science and technology. Unique facilities for energy-related R&D are used both for technology development and for fundamental investigations in the basic energy sciences that underpin the technology work. ORNL's scientific, engineering, environmental, economic, and social science expertise is integrated to supply the information needed in making decisions that ensure a sustainable energy future.



Computer visualization shows turbulent energy transport at small scales and large, "avalanche" scales. *Electronic file of Vickie Lynch's visualization enhanced by Allison Baldwin.*

A Sandpile Model for Fusion Plasmas

ORNL is using the model of a sandpile to better understand and control fusion plasma turbulence and energy losses.

To get electricity from a fusion reactor, you must heat charged particles (hydrogen nuclei) in a plasma to a high enough temperature and hold them close enough together using magnetic fields for a long enough time. If you do achieve the right plasma temperature, density, and confinement time, the hot nuclei will overcome their natural repulsion and fuse. Such fusion reactions release enormous amounts of energy that can be converted to electricity. But the energy required to sustain fusion reactions is often transported rapidly from the center of the plasma to the edge where it is lost. This undesirable loss of heat is caused by turbulence, the irregular fluctuations in plasma velocity and pressure brought on by the various mechanisms used to heat the plasma.

To better understand turbulent transport processes in fusion plasmas in the hope of controlling them, ORNL researchers Ben Carreras and David Newman are using an unusual model—a pile of sand. Imagine a child dumping a bucketful of sand on top of a sandpile at the beach. When the pile gets too high, it flattens out as avalanches occur, and the sand particles in the center are carried to the edge. The sandpile, a paradigm for self-organized criticality in which complex systems tend to rearrange themselves in a highly chaotic fashion, works especially well as a model for fusion in tokamaks, devices shaped like beach inner tubes. Hot particles pile up in the plasma center as the density and temperature peak, but the turbulence acts like sandpile avalanches, transporting hot particles from the center to the edge.

This new way of understanding turbulent transport processes in fusion plasmas offers possible explanations for universal transport behavior observed in many fusion experiments. These explanations in turn suggest techniques for controlling the performance of these experiments, making fusion as a future energy source more likely.

It was thought that hot particles move from plasma center to edge in random steps, like a staggering drunk. That suggested that the larger the tokamak fusion machine, the longer it would take for hot particles to carry their energy to the plasma edge. Experimental results, however, refute the theory that energy confinement time will be longer if the tokamak is larger. The results instead indicate that, if left uncontrolled, the transport of energy increases with size.

To minimize damage from large avalanches in a sandpile, the best solution is to perturb the sandpile a little, causing only small avalanches. In fusion plasmas, the way to minimize turbulence and its associated eddies is to introduce a radial electric field to apply a sheared flow to the plasma. Each eddy spanning the shear flow is forced to twist more in one direction so it can more easily "eat" its neighbor, causing a decrease in the size and connection of the eddies that can reduce the heat and particle loss. Experiments, in fact, show that when a shear flow is applied, energy transport is minimized and confinement of hot particles improves with tokamak size.

The principle of sandpile perturbations is also being applied to other situations. For example, synchronizing traffic lights to increase traffic flow may actually increase the chances of gridlock if a car blocks a lane because of a flat tire or a collision. Sandpile models suggest it might be better not to synchronize lights but, rather, create little, spaced-out traffic jams to decrease the probability of a larger jam later.

For large electrical grids, a blown transformer circuit could cause the rerouting of power, possibly overloading an alternate transmission line. To improve the reliability of power distribution and prevent major blackouts, it might be necessary to perturb the system a little, say, by occasionally manipulating circuit breakers.

For his work in applying the sandpile model to fusion energy, David Newman received a Presidential Early Career Award for Scientists and Engineers at the White House.

The work was sponsored by DOE's Office of Energy Research, Office of Fusion Energy Sciences.

ORNL Helps Design Superconducting Transformer

ORNL is working with several organizations to design a high-temperature superconducting transformer for industry.

As utilities replace aging and obsolete equipment, one improvement in the next 5 to 10 years is likely to be the high-temperature superconducting (HTS) transformer. This device, chilled by liquid nitrogen or a refrigerator, will offer several advantages over traditional paper-oil-insulated transformers wound with copper wire.

Transformers are needed at substations and on utility poles to step down high-transmission voltages and raise the current to levels needed for factories, offices, and homes. A transformer consists of two separate coils of insulated wire with different numbers of turns wound on an iron core. The alternating-current (ac) magnetic field created in one coil induces a current in the other coil in proportion to the number of turns. Coil windings are the source of more than 80% of the transformer's energy losses. Thus, DOE has long sought to develop more energy-efficient transformers.

Ben McConnell (left) and Bill Schwenterly shake hands to celebrate the ORNL team's success in completing the cryogenic winding assembly for the prototype 1-MVA superconducting transformer now being tested by Waukesha Electric Systems.

Unlike copper, HTS wires have no resistance to electrical flow. Hence, HTS transformers can greatly reduce heat losses in utility power systems and cut requirements for power generation. (Today's power transformers account for 50% of transmission system losses.) Because oil is a fire hazard and a potential contaminant whereas liquid nitrogen is nonflammable and environmentally benign, HTS transformers will be safer and more environmentally acceptable. In addition, HTS units do not require sprinkler systems and oil-containment devices, weigh less, and require less space, making them ideal for congested cities.

Today's transformers have reduced lifetimes if operated in an overload condition because their insulation is degraded by heat from fault currents and high continuous loads. Therefore, they are typically operated at less than 70% of their full capacity. In contrast, HTS transformers can take both momentary fault currents and continuous operation at their full rated capacity without damage. Using additional refrigeration, they can also accommodate continuous overloads without damage.

ORNL researchers are working with several organizations under a cooperative research agreement to help design an HTS substation transformer that will be acceptable to industry. Studies conducted by the team indicate that over its expected lifetime of 30 years, an HTS transformer's greater energy efficiency can more than pay for increased initial capital costs that arise from the more expensive conductor materials and the refrigeration needed to cool the coil to superconducting temperatures. Both the electric utility and manufacturing industries are seen as potential markets.

ORNL and its partners have built a 1-million-volt-ampere (1-MVA) prototype superconducting transformer that transforms 75 amps at 13.8 kilovolts to 150 amps at 6.9 kilovolts. The prototype is being tested at Waukesha Electric Systems in Wisconsin. Intermagnetics General Corporation near Albany, New York, helped design the cryogenic equipment, manufactured the superconducting coils by winding coils of wire (bismuth-strontium-calcium-copper oxide, or BSCCO-2212, on silver tape) on fiberglass forms, and shipped them to ORNL in January 1997. Waukesha Electric Systems provided the core, the bushings, and the vacuum tank. The utility partner, Rochester Gas and Electric Company in Rochester, New York, provided the utility perspective on many issues, such as the magnitude of fault currents and alternative methods of cooling (e.g., storing occasional truckloads of liquid nitrogen vs cooling with local refrigeration). The team also completed an economic analysis and preliminary commercial designs aimed at a 30-MVA rating.

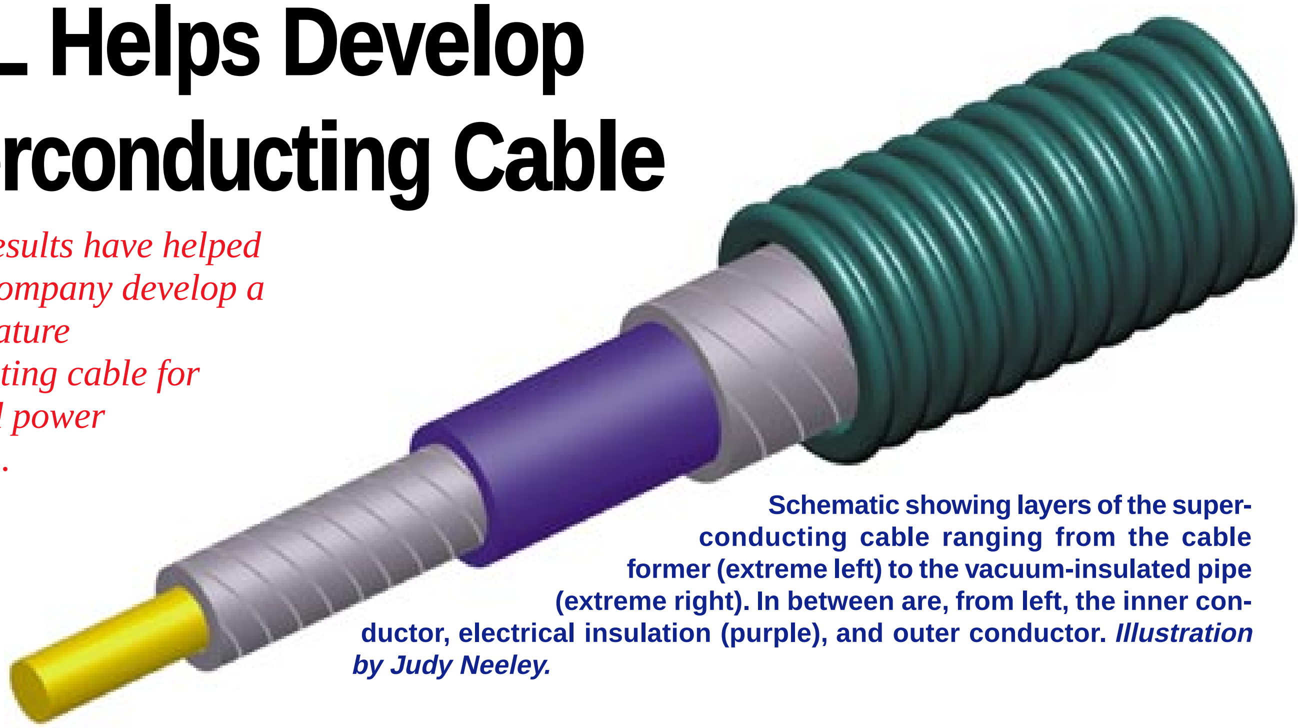
Because it is not beneficial to cool the iron core to the operating temperature of the coils, ORNL researchers designed a cryogenic suspension and cooling system to thermally isolate the chilled coil windings from the room-temperature laminated iron core. They assembled the bulk of the transformer, including the coils and their cooling piping, cryogenic suspension, 30-watt cryocooler, stainless-steel shield, and liquid-nitrogen tank.

The HTS transformer is likely to be more acceptable to utilities than low-temperature superconducting transformers developed in the 1970s and 1980s using helium-cooled niobium-titanium coils. Liquid helium is 100 times more expensive than liquid nitrogen, and these early devices could not handle fault currents properly. Today, utilities are offering warm support for the latest efforts toward developing the next generation of superconducting transformers.

The project was funded at ORNL by the DOE Superconductivity Program for Electric Systems.

ORNL Helps Develop Superconducting Cable

ORNL test results have helped Southwire Company develop a high-temperature superconducting cable for underground power transmission.



Schematic showing layers of the superconducting cable ranging from the cable former (extreme left) to the vacuum-insulated pipe (extreme right). In between are, from left, the inner conductor, electrical insulation (purple), and outer conductor. *Illustration by Judy Neeley.*

A shift in the "underground power structure" in large cities may be around the corner. Electrical power delivered underground in cities normally flows through traditional copper cables in 20-centimeter ducts. But as these aging cables need to be replaced, utilities may be attracted to high-temperature superconducting (HTS) cables in the next decade. Here's why.

An HTS cable offers very little resistance to electrical flow, so it loses little energy in the form of heat during transmission. Thus, a superconducting cable carries three to five times as much electrical current as a traditional copper cable the same size. Utilities can use existing rights-of-way and ducts for new HTS cables. Superconducting cables are more environmentally friendly because they are cooled with safe and inexpensive liquid nitrogen rather than by oil-impregnated paper insulation, which sometimes leaks oil.

The demand for underground HTS cables that can carry double the current of conventional copper cables is expected to grow into a multimillion dollar industry between 2005 and 2020 for several reasons. New construction techniques will cut the costs of installing underground transmission cables as securing rights-of-way for overhead lines becomes more difficult. Underground cables are safer than overhead lines and, because they are hidden, do not contribute to visual pollution. Because fewer superconducting cable circuits are needed to transfer power, they will take up less space and will be easier and cheaper to install. HTS cables also will be able to transmit alternating current (ac) much longer distances than underground copper cables, which are limited to less than 20 miles because of the cable capacitance.

A dozen ORNL researchers are helping Southwire Company in Carrollton, Georgia, design a first-generation, high-temperature superconducting cable that may be used for underground transmission in metropolitan areas and over long distances. In its fusion energy facilities, ORNL has tested nine 1-meter-long HTS cables manufactured by Southwire to determine the amount of current they can carry and the extent of ac losses (based on heat generated, as measured by thermocouples). In another ORNL lab, researchers are testing the ability of the cable's electrical insulation to withstand lightning strikes and switching surges at liquid nitrogen temperatures and pressures; they measured the voltage levels at which holes are punched in the insulation so they could determine the maximum voltage levels that must be accommodated in the design to reduce the risk of short circuits. Results of the ORNL tests have influenced the final cable design.

The HTS cable consists of tapes made by packing bismuth-strontium-calcium-copper oxide (BSCCO) powder in silver tubes and stretching and flattening the tubes into tapes. Southwire has teamed with Intermagnetics General Corporation in New York to develop these BSCCO tapes. ORNL researchers have been measuring the critical current of the BSCCO tapes and the effect of strain tolerance upon the critical current.

The cable is made on a hollow tube called cable former through which liquid nitrogen flows (see figure above). Southwire plans to use a 38-millimeter former over which HTS tapes will be wrapped to make the inner conductor, which carries the cable's electricity. The wrapped tube is surrounded by Southwire's proprietary electrical dielectric tape, called Cryoflex. This electrical insulation is wrapped in BSCCO tapes to form the shield conductor, which prevents external magnetic fields (say, from parallel cables) from destroying the inner conductor's superconducting properties. The outermost part of the cable is the vacuum-insulated pipe, providing thermal insulation to keep the inner temperature of the cable near 77 K.

After ORNL completes a variety of tests of 5-meter-long HTS cables in a single facility in 1998, Southwire will install a 30-meter (100-foot) cable to provide power from its local utility to two manufacturing plants at its Carrollton complex. The 12.5-kilovolt, 1250-ampere HTS cable will be demonstrated by the end of 1999. If officials of electrical utilities like what they see, our infrastructure may soon be wired in a different way to bring power to the people.

The project is funded by DOE's Office of Energy Efficiency and Renewable Energy, Office of Utility Technologies.

Prototype catalytic converter installed in engine test cell at Advanced Propulsion Tech Center. ***Digital image enhanced by Allison Baldwin.***

Studying NO_X Catalysts for Efficient Cars

ORNL is helping to characterize novel catalysts and their effectiveness in reducing nitrogen oxide emissions from highly efficient diesel cars of the future.

The lean, clean car of the future proposed by the U.S. Partnership for a New Generation of Vehicles (PNGV) may have an improved diesel engine. This compression-ignition, direct-injection (CIDI) engine today uses 35 to 40% less fuel per mile than gasoline-burning, spark-ignition engines typical of most cars. Because PNGV's goal is to design and produce a car by 2004 that has a fuel efficiency of up to 80 miles per gallon, the CIDI engine is a prime candidate for this vehicle. A second DOE program seeks to clear the way for diesel engines to be used in light trucks and sport utility vehicles to improve their fuel economy by over 35%.

The challenge of today's diesel engines is their high emissions of nitrogen oxides (NO_x) and particulates. NO_x is undesirable environmentally because it contributes to the formation of smog and acid rain. Diesels present a particular NO_x dilemma because their lean-burn operation is incompatible with today's highly effective exhaust aftertreatment catalytic converters that eliminate about 90% of the NO_x from today's cars. Hence, a new type of exhaust catalyst system is needed.

DOE national laboratories (including ORNL) are helping to develop new NO_x control systems specially suited to the diesel engine. They are working with Chrysler, Ford, and GM (through the United States Council for Automotive Research, or USCAR), as well as diesel engine manufacturers, such as Cummins and Detroit Diesel Corporation, under cooperative research and development agreements (CRADAs). Ron Graves has led ORNL's development of CRADAs with engine manufacturers that complement our work with the auto companies.

The search is on for a catalyst that selectively adsorbs NO_x from the exhaust gases passing through the catalytic converter and then chemically reduces the NO to N_2 in an oxidizing atmosphere. For the diesel-propelled car or truck, the new catalyst systems may incorporate either precious metals or metal oxides.

Our role is to apply broad analytical and experimental capabilities to evaluating the performance of the new catalysts. Using electron microscopes, our materials scientists are characterizing the microstructures of these catalysts (e.g., the spatial distribution of platinum atoms or the movements of rhodium atoms) to better understand how they perform. Our engineers, chemists, and physicists at the Advanced Propulsion Tech Center (at the Oak Ridge Y-12 Plant) are identifying and quantifying the constituents of diesel engine exhaust before and after it passes through the catalytic aftertreatment device. Gas chromatography, mass spectrometry, and Fourier transform infrared spectroscopy are used to determine if a test catalyst effectively removes NO_x from the exhaust. One finding is that, for diesel fuel, precious-metal catalysts work well below the desired temperature and metal-oxide catalysts work well above the desired temperature, suggesting that the best aftertreatment may involve the combined use of both catalyst types.

At the ORNL diesel engine test stand, researchers are studying the hydrocarbons from the engine's unburned diesel fuel that may enhance the catalyst's performance. The hydrocarbons react with the nitrogen oxides, converting them to nitrogen, carbon dioxide, and water vapor. ORNL researchers are evaluating techniques that may enable the introduction of the right hydrocarbons to the exhaust system at the right time to optimize the performance of the chosen catalyst.

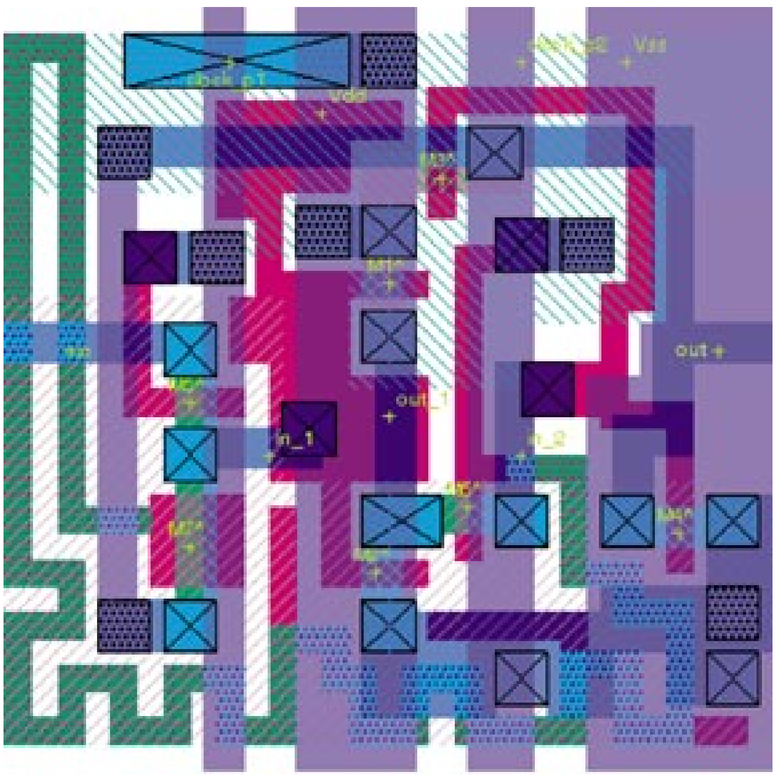
For the PNGV work, ORNL researchers led by Ralph McGill and their partners from other DOE laboratories and industrial firms received a PNGV Award for technical accomplishment and teaming for lean-burn NO_x catalyst research. But the best prize will be the development in time of a near-zero-emission, energy-efficient car.

The research has been funded by DOE's Office of Energy Efficiency and Renewable Energy, DOE's Defense Programs, and our CRADA partners.

Norberto Domingo and Karren More discuss the ability of the materials in the aftertreatment device catalyst (held by Domingo) to remove nitrogen oxides from diesel engine exhaust. ***Photograph by Tom Cerniglio.***

Instrumentation and Measurement Science and Technology

In 1997, ORNL made some exciting advances in the development of instruments. We helped develop the "critters on a chip" technology, a living electronic sensor in which bacteria light up in the presence of specific chemicals, such as pollutants in soil. We have devised a highly sensitive and selective hand-held DNA biochip system that may someday diagnose patients' diseases rapidly in the doctor's office. We are developing a chip writing system using electron beams to make faster silicon wafers for computers. Our newly developed "blend-down" monitor is helping to verify that Russian weapons-grade uranium is being converted to reactor-grade uranium fuel, extending energy supplies while cutting back on weapons material.



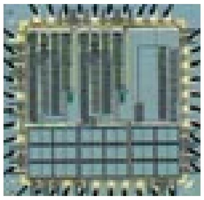
Layout for a logic chip.

To address national needs for improved measurement, monitoring, and control systems, ORNL has broad R&D capabilities in the physical, chemical, electronic, engineering, and computational sciences that can be combined to provide a powerful institutional capability. Our particular strengths include microelectronics and photonics; signal processing and simulation; analytical chemistry and chemical physics; materials characterization; robotics and intelligent systems; and sensors for physical, chemical, biological, and radiological phenomena.

Our activities include fundamental research for elucidating principles that enable novel advances in the measurement sciences; applied research that improves the accuracy, sensitivity, cost-effectiveness, and practicality of advanced techniques and prototype instruments; and design, fabrication, and installation of one-of-a-kind devices and systems. Integration of these capabilities allows the definition, design, and implementation of new instruments and methods for a variety of ORNL activities: energy production and manufacturing processes, environmental characterization and remediation, biotechnology and human health, and national security and forensic science. At the same time, this area of emphasis enhances ORNL's ability to obtain, process, and analyze the research data needed to support DOE's science missions.

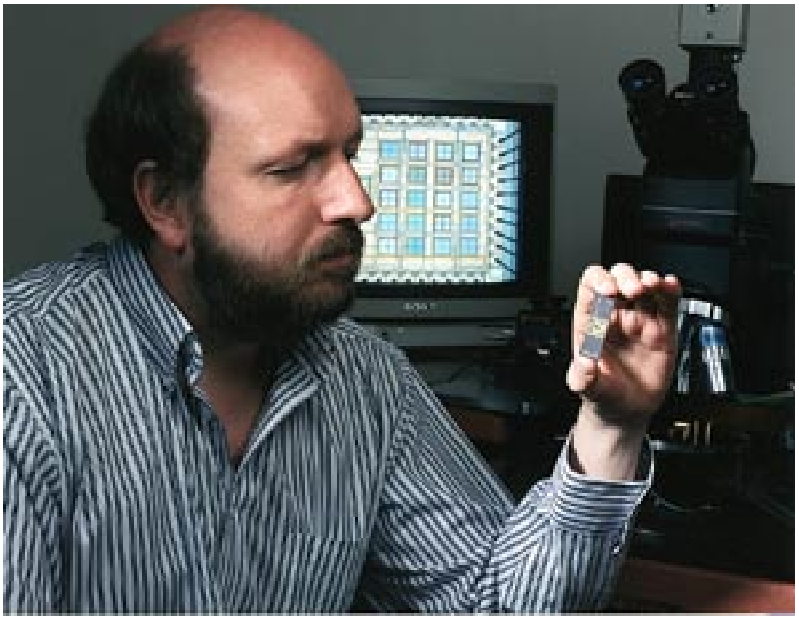
"Critters on a Chip" Detect Pollutants

ORNL helped develop a living electronic sensor in which bacteria light up in the presence of specific chemicals.



A silicon chip the size of a match tip is deposited in a contaminated environment. Bioluminescent bacteria intentionally placed on the chip begin to "eat" the pollutant. As the living cells enjoy their feast, they light up. Their photons of blue-green visible light are absorbed by the silicon, creating electrical charges that are fed into processing circuitry on the chip. Signal-processing microelectronics measure the tiny electrical current and sound an alarm. The "critters on a chip," which were genetically engineered to emit light as they eat and digest environmental pollutants, have indeed detected naphthalene and toluene. And the chip electronics linked to these living sensors reveal the concentration of each pollutant, which is related to the amount of electric current produced.

The critters-on-a-chip technology developed at ORNL in 1996 could be used to map soil contamination (by sprinkling a suspect area with the tiny chips). A prototype device was made at ORNL by coupling *Pseudomonas fluorescens* HK44, a novel naphthalene bioreporter microorganism developed by the University of Tennessee Center for Environmental Biotechnology (UT-CEB), to an optical application-specific integrated circuit (OASIC) developed at ORNL. A measured electrical signal was obtained when the device was exposed to moth balls, which are made of naphthalene. A second prototype used the toluene-sensitive *Pseudomonas Putida TVA8*, also developed at UT-CEB.



Mike Simpson examines the bioluminescent bioreporter chip (magnified on the monitor in the background). Genetically engineered bacteria on the chip emit blue-green light when the pollutant is detected. The chip detects this light. *Photograph by Tom Cerniglio.*

The combination of the OASIC chip and bacteria engineered to be sensitive to a specific biological or chemical agent could have many applications. The technology could be used to detect specific chemicals in groundwater or soil, including liquid pollutants from fuel spills, toxic metals such as mercury, and explosives such as TNT that may have leaked from land mines. Oil exploration companies might want to use it to detect hydrocarbons that indicate the presence of nearby oil and gas deposits.

Because of the technology's exciting uses and because of the catchy nickname "critters on a chip" coined by chip developer Mike Simpson of ORNL to better promote the concept, the news media have had a field day with it. It has been featured on television and National Public Radio, and articles on the technology have appeared in *Christian Science Monitor, New Scientist, National Geographic*, and *Business Week*.

As a result of the *Business Week* article, Perkin-Elmer Corporation is developing the chip with ORNL and UT through a $4.05 million cooperative research and development agreement.

The concept sprouted in the summer of 1996 after Simpson heard a seminar on bioremediation given at ORNL by Gary Sayler, UT-CEB director and UT professor of microbiology and ecology. Sayler mentioned successes in incorporating a gene into the bacterial genome that makes the one-celled organism emit visible light during metabolism of its favorite nutrient. One gene (which codes for luciferase) comes from fireflies, and the other gene comes from the bacterial genus *Vibrio*, whose members get protection on a deep-sea fish species in exchange for emitting light the fish needs to attract prey or a mate.

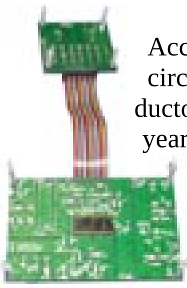
After the talk, Simpson approached Sayler, saying, "You engineer bacteria to emit low levels of light, and I develop optical sensor chips that detect low levels of light. Perhaps we should do a project together."

The rest is history. It is now possible to make living sensors using integrated-circuit chips that are small and rugged and require little power. Such wireless chips can be deployed where other devices can't (e.g., groundwater, industrial process vessels, and the battlefield). The key is to place the bioreporter bacteria on a transparent silicon nitride film that protects the etched silicon chip from damage in the presence of hazardous chemicals. To increase the shelf life of the bioreporter chip, the bacteria could be freeze dried, and a micromachine on the chip could activate the living sensors when needed by "dumping" water and nutrients on the dormant bacteria. The chip can be configured to transmit a signal to a receiver linked to a computer. The technical people on the project now call the hybrid, half-living, half-silicon devices "bioluminescent bioreporter integrated circuits," but most folks prefer to call them "critters on a chip."

DOE's Laboratory Technology Research Program helps fund this work.

Digital Electron Beam Technique May Make Faster Silicon Chips

ORNL is developing a chip-writing system using electron beams to make faster silicon wafers for computers.



According to Moore's law, the circuit density on a semiconductor chip doubles every two years and the computing speed resulting from jamming more circuits on each chip doubles every 18 months. To help uphold this law, 10 ORNL electrical engineers and physicists are developing a chip-writing system using electron beams. This system is designed to cram more transistor circuits into the same amount of chip space. By reducing the distances that electrons must travel, this system would make chips that make more calculations faster while using less power—just what the semiconductor industry is seeking. Such chips are needed to speed up computers and other electronic devices.

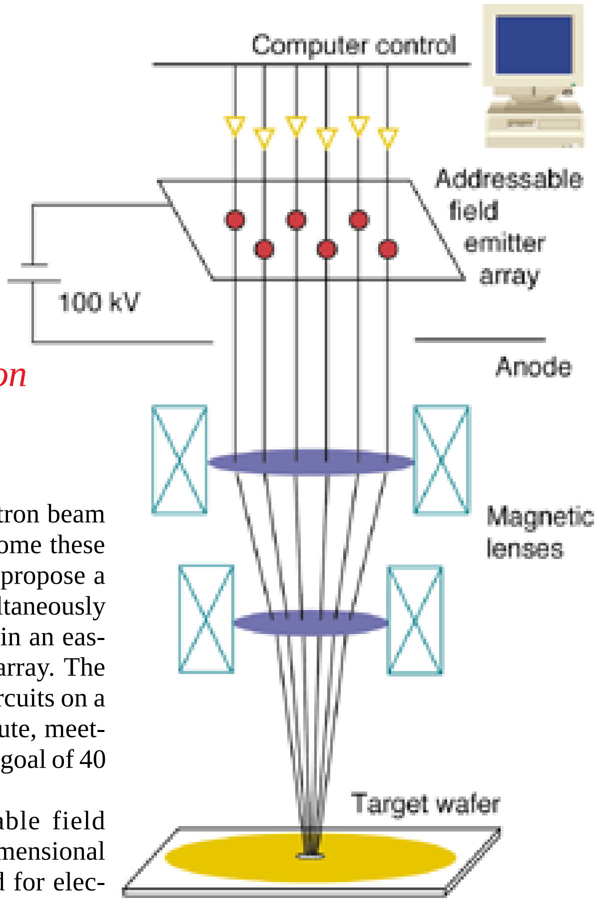
Today's integrated circuits are etched on chips by use of light—optical lithography. A mask containing a circuit pattern is imaged on a silicon chip, and a beam of light exposes the photoresist in the chip part not shielded by the mask. The size of circuits made by optical lithography is limited by the wavelength of light. Because the electron wavelength is so much shorter, an electron beam could carve a much narrower winding path in the chip, creating a finer, more closely packed circuit. Today's state-of-the-art circuits are about 200 nanometers (nm) wide, but ORNL researchers in six divisions, led by C. E. (Tommy) Thomas, think their technique could make a circuit only 100 nm across. They believe that by 2004, they will meet the semiconductor industry's goal of making production chips whose circuits are 8 times denser and up to 16 times faster than chips of the same size currently being etched by optical lithography.

Although electron beam technology has long been a strong candidate for chip lithography, writing with a single electron beam is slow and expensive. To overcome these deficiencies, ORNL researchers propose a maskless system that writes simultaneously with millions of electron beams in an easily programmable field emitter array. The system should be able to write circuits on a 300-cm^2 (8-inch) wafer in a minute, meeting the semiconductor industry's goal of 40 to 80 wafers an hour.

ORNL's proposed addressable field emitter array (AFEA) is a two-dimensional array of miniature cathodes used for electron beam sources. The proof-of-principle AFEA chips developed at ORNL have 5-micron cathodes 300 microns apart, but the researchers believe that, with the aid of an industrial partner, 200-nm cathodes can be made for chip writing (250-nm circuits are present on Intel's fastest Pentium chips). ORNL's goal is an array of 6.25 million (2500 × 2500) 200-nm cathodes on a 1-cm chip.

Using laser ablation, ORNL solid-state physicists have formed cathodes from amorphous diamond deposited on the array. When a computer-controlled bias grid places a cathode under a voltage, it emits electrons, which are accelerated to 100 kilovolts to avoid aberrations caused by stray magnetic fields. When the voltage is dropped to zero, the cathode stops emitting electrons.

Each cathode is addressable by a computer, enabling the programming into the AFEA of the desired circuit patterns to be written onto the target chip. The chip-writing program will be allocated to a network of 100 parallel computers (taking up the space of an office desk), which will send turn-on and turn-off signals to the AFEA logic and memory circuits connecting the cathodes. This digital "mask" can be reprogrammed to create different circuits on new layers within milliseconds.

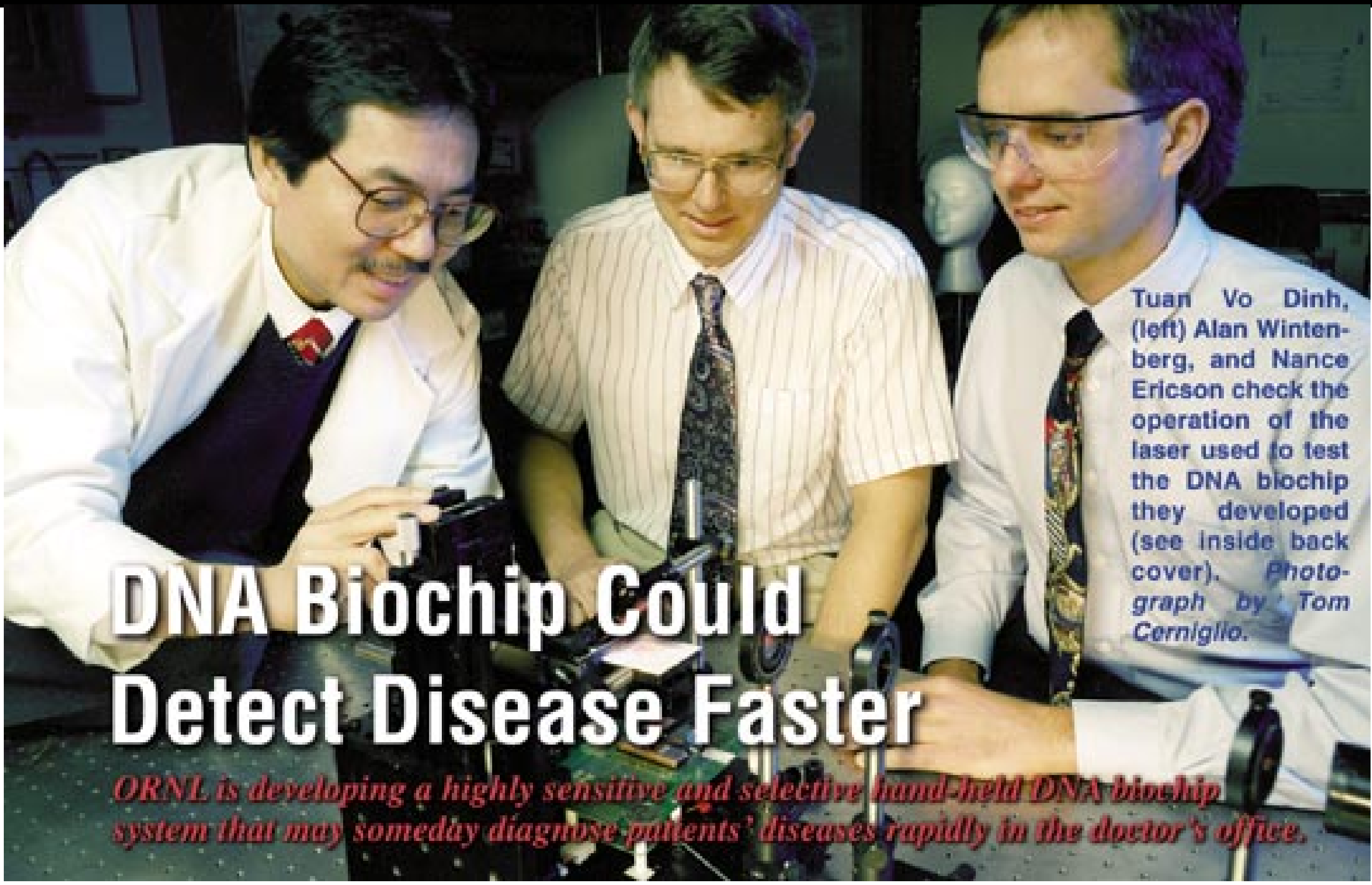


Schematic of ORNL's proposed chip-writing system.

Because ORNL researchers are facing competition from other techniques being developed (which use extreme ultraviolet light, laser light, X rays, or electron beams using masks), they are working vigorously to tackle various technical issues to make the system work. They will determine if amorphous diamond nanocathodes are reproducible and if they can be made stable and reliable enough to operate for months at a time. They will try to scale up the magnetic lens to focus into a "writing" beam the individual beams of electrons in a much larger array than is currently being handled by the best electron microscopes.

ORNL's proof-of-principle AFEA chips are assembled by IntraSpec of Oak Ridge. In 1998 the researchers will test many 2-millimeter chips, each with an array of 25 amorphous diamond cathodes (5 × 5). It may be the start of the chip-writing system of the future for the semiconductor industry, one that would show that Moore's law still holds true.

The development is being supported by the U.S. Defense Advanced Research Projects Agency.



DNA Biochip Could Detect Disease Faster

ORNL is developing a highly sensitive and selective hand-held DNA biochip system that may someday diagnose patients' diseases rapidly in the doctor's office.

Tuan Vo Dinh, (left) Alan Wintenberg, and Nance Ericson check the operation of the laser used to test the DNA biochip they developed (see inside back cover). *Photograph by Tom Cerniglio.*

You're coughing and feeling weak. You make an appointment with your doctor. A nurse greets you in the office waiting room, takes a drop of blood from your finger, and injects the blood into an instrument that fits in the palm of her hand. When you see the doctor ten minutes later, you learn the results. You don't have tuberculosis (TB) or the AIDS virus or any signs of genetic predisposition to cancer. You just have a bad case of the flu.

In two or three years, physicians may be making rapid diagnoses of patients' conditions using a small instrument containing a DNA biochip like the one being developed at ORNL by Tuan Vo-Dinh, Alan Wintenberg, and Nance Ericson. A DNA biochip mimics a living system's sophisticated recognition capability, making it highly selective and sensitive; it is able to distinguish between, for example, a bacterium and a virus or between a chemical and a biological organism.

The DNA biochip developed at ORNL will provide results in minutes instead of a few days, as is commonly the case when blood samples are sent to the laboratory for analysis by gel electrophoresis. In addition, a DNA biochip requires less blood for analysis. Unlike gel electrophoresis, the DNA biochip system uses no radioactive substances. Thus, it does not pose potential health risks for technicians handling samples, use materials that have a short shelf life, or have high disposal costs.

ORNL researchers have demonstrated the concept of a miniaturized DNA biochip system using a laser, an electric-optic integrated-circuit chip, an amplifier, and other electronics. Aided by Jean Pierre Alarie, Narayan Isola, and David Landis, Vo-Dinh showed that the concept works on a synthetic gene fragment of the AIDS virus. Other probes they designed for testing are a synthetic TB bacterium and cancer genes.

ORNL's thumbnail-size biochip will contain a membrane on which are bound up to 100 different DNA fragments. Each fragment consists of a characteristic order of chemical bases, or "letters," that spell out part of a gene [adenine (A), thymine (T), guanine (G), cytosine (C)]. Some of these bound fragments may be "detected" by free DNA probes that are introduced to the membrane. Because base A always pairs with base T and base G always pairs with base C in opposite strands of DNA (e.g., AACCT pairs with TTGGA), the free DNA probe will attach, or hybridize, itself to the bound DNA fragment that has the right opposite bases in the same sequence. The two strands are said to be complementary to each other.

For example, here's how the biochip could determine if a patient has the AIDS virus. DNA fragments isolated from a patient's blood are bound chemically on the biochip's membrane. DNA probes tagged with a fluorescent dye that are complementary to pieces of the AIDS virus DNA are introduced, and, following an amplification process, the tagged DNA attaches to any DNA present on the membrane to which it is complementary. The unattached free DNA is washed off. A laser light illuminates the membrane, causing the attached tagged DNA to give off light, which is captured by detectors below the membrane and turned into electrical signals that provide the diagnosis to the doctor.

Following system packaging, clinical trials could begin to test the device for biomedical applications. If everything goes smoothly, in about two or three years, the DNA biochip system could be in use to give patients and doctors results in only a few minutes. Such a device could help doctors diagnose important diseases earlier, cutting health care costs.

ORNL's Laboratory Directed Research and Development Program and DOE's Office of Biological and Environmental Research sponsored this work.

Confirming Conversions of Weapon Materials to Reactor Fuels

An ORNL-developed instrument is helping to verify that Russian weapons-grade uranium is being converted to reactor-grade uranium fuel.

Reducing the number of nuclear weapons in the world is one of President Clinton's chief foreign affairs goals. One step toward achieving that goal is the U.S. purchase of 500 metric tons of highly enriched uranium (HEU) from the Russian Federation over the next 20 years at a cost of $12 billion. The HEU extracted from nuclear weapons is being diluted, or blended down, in Russia to produce low-enriched uranium (LEU) for use as fuel for nuclear reactors that generate electricity. In this way, the uranium in weapons cannot be recycled to make other weapons, but it can be used to extend each nation's uranium supplies for energy production. An instrument developed at ORNL will be one of two used to verify that the Russians have properly blended down the 500 metric tons HEU purchased by the United States.

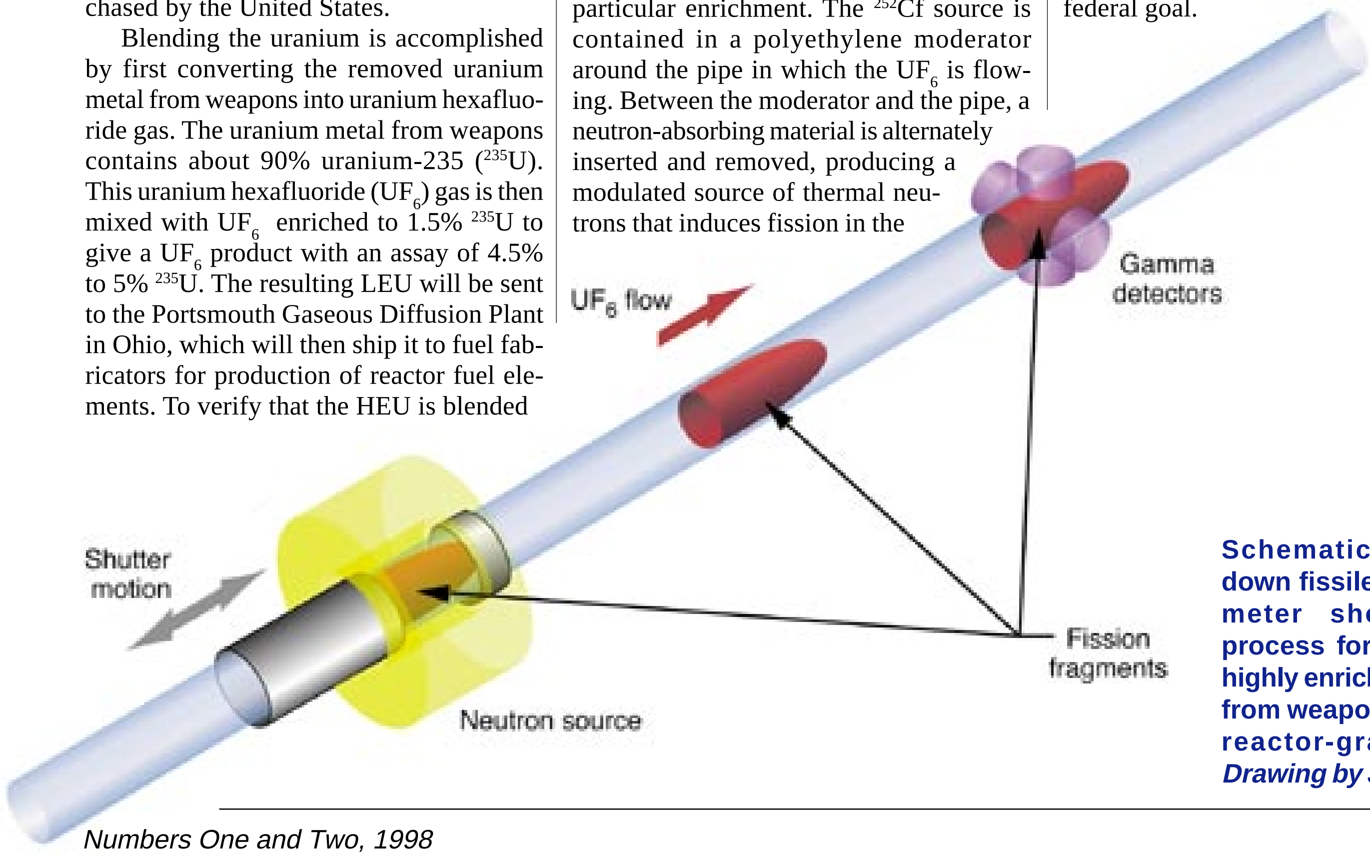
Blending the uranium is accomplished by first converting the removed uranium metal from weapons into uranium hexafluoride gas. The uranium metal from weapons contains about 90% uranium-235 (^{235}U). This uranium hexafluoride (UF_6) gas is then mixed with UF_6 enriched to 1.5% ^{235}U to give a UF_6 product with an assay of 4.5% to 5% ^{235}U. The resulting LEU will be sent to the Portsmouth Gaseous Diffusion Plant in Ohio, which will then ship it to fuel fabricators for production of reactor fuel elements. To verify that the HEU is blended down, a special measurement system that could be deployed without cutting pipes was needed.

To meet this requirement, an ORNL team led by John Mihalczo, Jim Mullens, and Jose March-Leuba developed, tested, demonstrated, and implemented the blend-down fissile mass flowmeter. A prototype was demonstrated to DOE and the Department of State and to representatives of the Russian Ministry of Atomic Energy. The United States has negotiated the installation of this equipment in Russian facilities involved in the blend-down of HEU as a way to provide confidence that the Russian Federation is abiding by terms of the agreement.

The flowmeter contains a californium-252 (^{252}Cf) source that introduces neutrons periodically into the pipe carrying UF_6 of a particular enrichment. The ^{252}Cf source is contained in a polyethylene moderator around the pipe in which the UF_6 is flowing. Between the moderator and the pipe, a neutron-absorbing material is alternately inserted and removed, producing a modulated source of thermal neutrons that induces fission in the UF_6 gas, producing waves of activation (delayed gamma ray emissions by uranium atoms in the gas along the pipe) that are detected downstream. The time delay between the activation and the detection downstream, and the distance between the source and detectors, allows measurement of the gas flow velocity. The amount of the signal downstream at the detector is proportional to the concentration of ^{235}U in the gas. (The more uranium, the more gamma rays in the signal.) From these two quantities, the fissile mass flow is obtained.

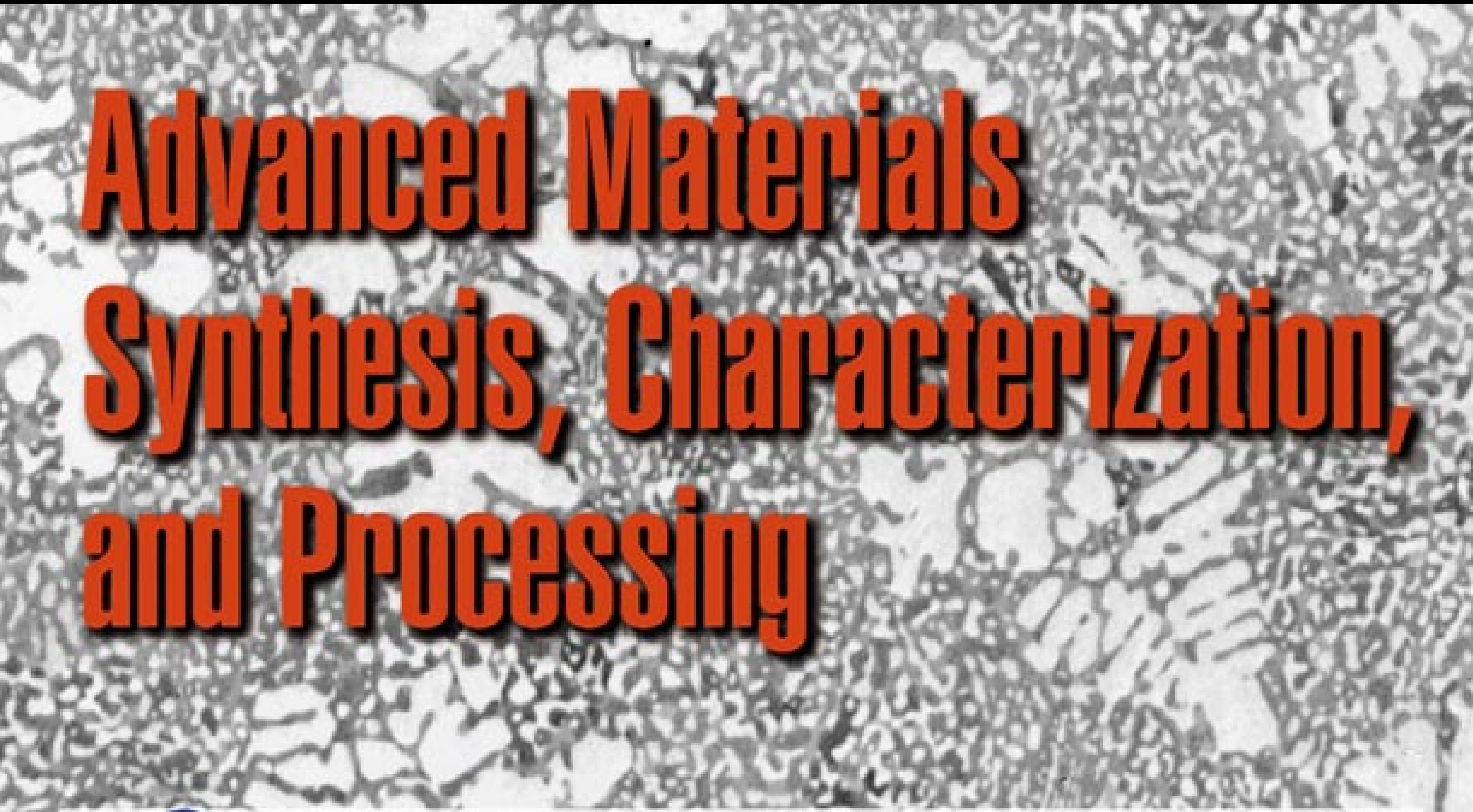
The blend-down fissile mass flowmeter is undergoing calibration and verification demonstrations with 1.5 wt % ^{235}U-enriched gas at the Paducah Gaseous Diffusion Plant. It will be installed in Russia to monitor blend-down of the U.S.-purchased uranium. The flowmeter has been demonstrated to Russians as part of their training so that they can safely install and operate it at the Russian blend-down facilities. Jim McEvers and William H. Sides are project managers for the fabrication and installation of the flowmeter in Russia.

This program has brought international recognition to ORNL. The Laboratory received a substantial amount of funding for the development of this instrument for use in the Russian blend-down facilities. While reducing nuclear weapons-grade uranium, the ORNL instrument is helping the United States extend its supplies of nuclear fuel for power production, helping meet yet another federal goal.



Schematic of blend-down fissile mass flowmeter showing the process for converting highly enriched uranium from weapons-grade to reactor-grade fuel. *Drawing by Judy Neeley.*

Advanced Materials Synthesis, Characterization, and Processing



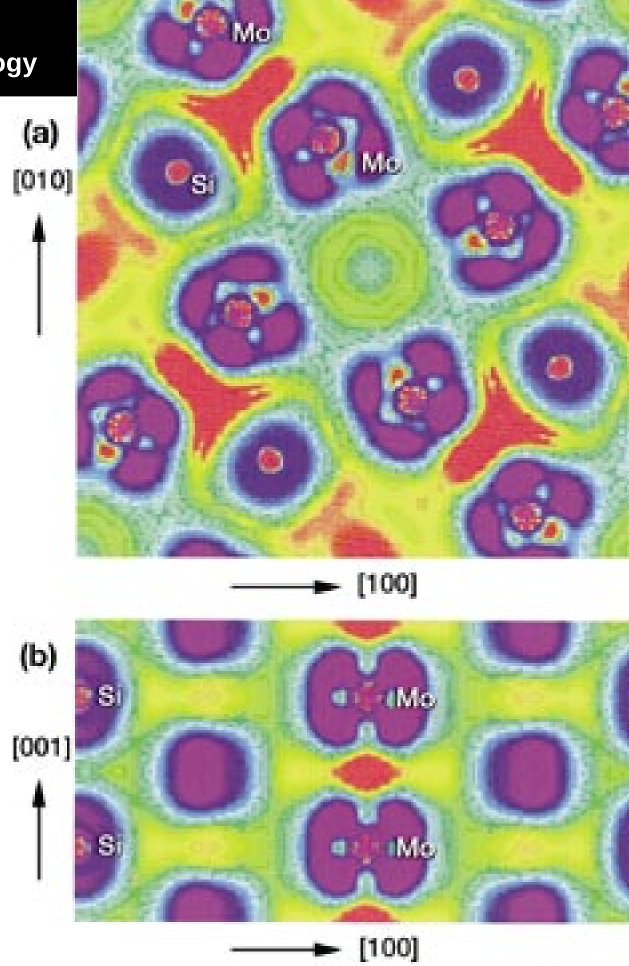
ORNL is a world leader in materials science and technology. Our strengths in advanced materials R&D support the development of ceramics and composites, metals and alloys, surfaces and thin films, polymers, superconductors, and new techniques for materials processing and characterization. This work advances the materials frontier and provides the underpinning for technologies that support DOE's energy resources mission. Notable characteristics include the integration of basic and applied research, unsurpassed characterization facilities, extensive synthesis and processing capabilities, and broad partnerships with industry.

In 1997 ORNL's modified infrared camera imaged hot spots on auto disk brake rotors that could lead to a better brake design and cut the auto industry's warranty costs. In solid-state physics theory, we broke new ground with predictions of "magic numbers" that are linked to the growth of ultrathin metallic films on semiconductors; the theory offers a different approach to growing smooth metal films on semiconductors for possible use in advanced electronic devices. ORNL-developed nickel aluminides sold well, thanks to several additional licenses of the technology. We made important strides in working with our partners to modify molybdenum silicide to make it tougher for use in high-temperature turbines and other applications. ORNL, Sandia National Laboratories, and Idaho National Engineering and Environmental Laboratory have been developing and testing hybrid techniques for welding steels and directly fabricating tools and dies in Lockheed Martin Corporation's System of Labs approach to helping American industry become more competitive.

A mixture of two phases is shown in this micrograph of the microstructure of a cast molybdenum silicide alloy heat treated for 150 hours at 1400°C. White particles represent the soft molybdenum-rich phase and the gray matrix is a hard molybdenum-silicide phase. A unique mixture of both soft and hard phases provides a good resistance to cracking and fracture for this in-situ composite material.

ORNL Successes in Intermetallics

ORNL-developed nickel aluminides are selling well, and ORNL is helping to make molybdenum silicide tougher for use in high-temperature turbines.



The calculated bonding charge density shows the depletion of density at the lattice sites (purple) together with an increase of density in the interstitial region. The bonding has pronounced covalent components (red), characterized by (a) the planar Mo-Si-Mo triangular bonding units on the (001) plane, and by (b) the unusually short Mo-Mo bond along the c axis. These covalent bonds give rise to the alloy's strength.

Now that some manufacturing firms recognize that nickel aluminide (Ni_3Al) alloys last much longer than commonly used materials under typical industrial conditions, commercial sales of Ni_3Al alloys based on ORNL compositions continue to rise. They exceeded 100 tons in 1997, and licensees expect sales to reach almost 250 tons in 1998. The chief reason for the climbing sales is the addition of six new licenses since 1995, bringing the total number of active nickel aluminide licensees to eight. (The total number of licenses signed is 13, but 5 have been terminated.)

Ni_3Al alloys are being used in dies for making truck brake parts and tools like pliers and wrenches. A major steel company is replacing its steel transfer rollers with Ni_3Al rollers, which are used to move steel plates through a furnace where they are softened for shaping into structural components. The steel and automotive industries are beginning to show interest in replacing their radiant burner tubes with tubes made of Ni_3Al. These tubes of burning gas are used in industrial furnaces for heat-treating parts to harden their surfaces. Because Ni_3Al lasts much longer in a furnace's carbon atmosphere than conventionally used materials, it is expected to be used increasingly in industrial heat-treating equipment.

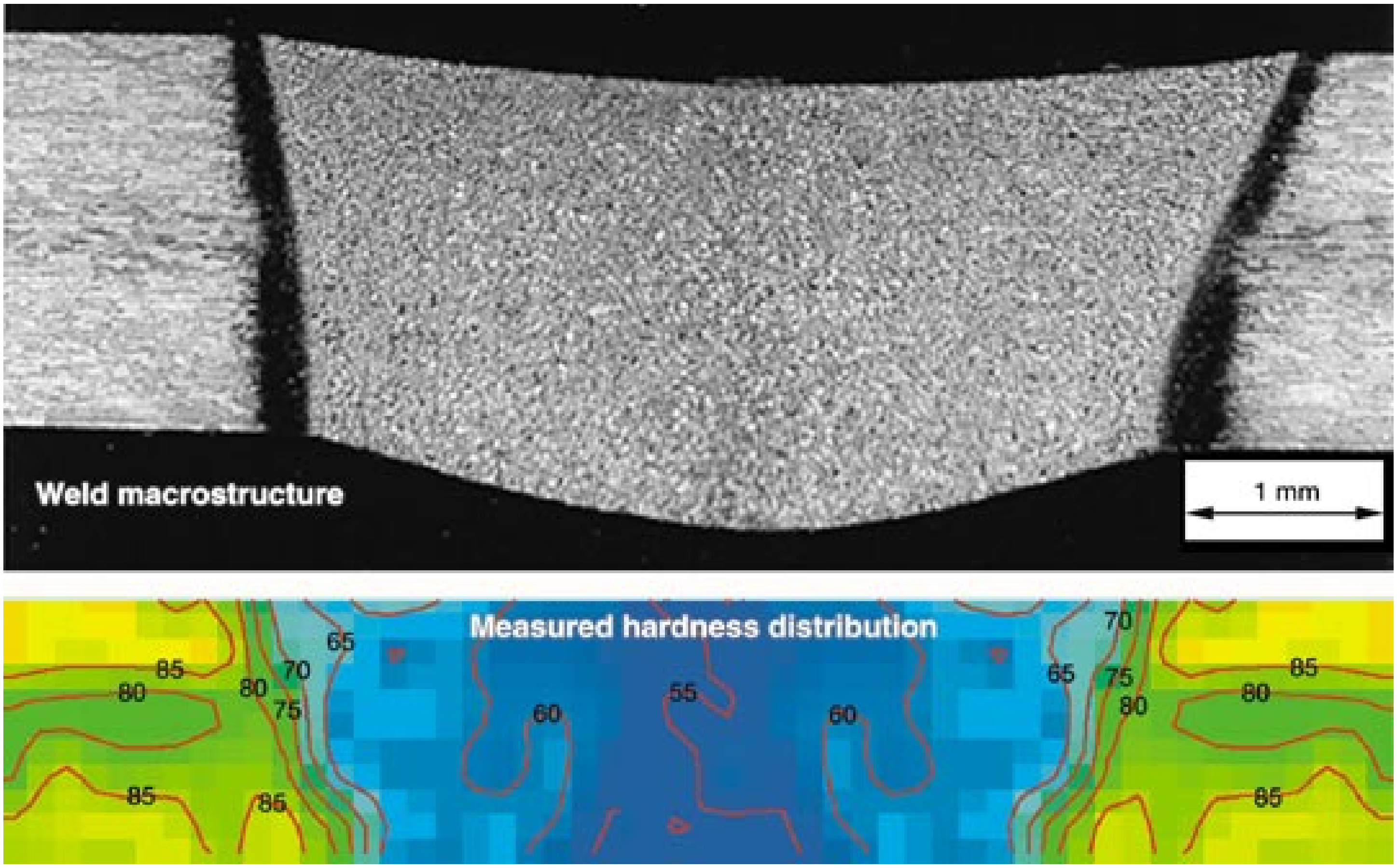
The success of ORNL's intermetallics research and development programs and the commercialization of this technology under DOE's Office of Energy Efficiency and Renewable Energy, Office of Industrial Technology, Advanced Industrial Materials Program, was confirmed in a recent evaluation by the National Materials Advisory Board of the National Research Council. This report acknowledges the quality of both the research and the management of the intermetallics program.

New research directions at ORNL in intermetallics include development of ultrahigh-temperature intermetallic silicides. Today, intermetallic alloys such as Ni_3Al alloys can be used in devices that operate at 1200°C, but alloys that can operate above 1300°C are needed for advanced turbine blades, heat exchangers, advanced coal conversion plants, and high-temperature glass-molding devices. Molybdenum silicides have excellent strength and creep resistance above 1300°C, but they are brittle at ambient temperatures and not resistant enough to fracture to be used as structural engineering materials. Research to improve the properties of silicides was approved in April 1997 as a project of the DOE Center of Excellence for the Synthesis and Processing of Advanced Materials sponsored by DOE's Division of Materials Sciences. Center projects involve collaborative research among a number of national labs. The project also has support from DOE's Fossil Energy Materials Program and Advanced Industrial Materials Program.

ORNL has the technical lead for developing molybdenum silicide alloys with Ames Laboratory, which discovered that the addition of boron improves the alloys' oxidation resistance. Rod Judkins is project coordinator and C. T. Liu is technical coordinator for the ORNL part of the effort.

At ORNL C. L. Fu is leading the theoretical effort on first-principles calculations for the electronic and structural properties of molybdenum silicides. Collaborating theorists at ORNL and Ames Laboratory have already investigated phase stability, bonding strength, elastic properties, and thermal expansion coefficients in the alloy. The bonding in this alloy was found to be covalent, which gives rise to the strength of this material. The calculated elastic constants agree with experimental measurements at Los Alamos National Laboratory.

ORNL experimenters Liu, Joachim Schneibel, and Easo George studied multiphase alloys based on Mo_5SiB_2, which shows good creep resistance and oxidation resistance at high temperatures. They found that the alloy's oxygen resistance is sensitive to its silicon level. They studied the effects of oxygen and carbon impurities on the silicide and determined the alloy's microstructure, alloying effects, mechanical behavior, interfacial properties, and criteria for material processing. In this multiyear project, they hope to solve technical problems such as making the alloy less brittle and tougher by incorporating additives in the right proportions, controlling interfacial structures and properties, making the cast structure less porous, optimizing the alloy's microstructure to get good mechanical properties, and improving the alloy's oxidation resistance at high and low temperatures. Already the experimental program's multiphase alloying approach has resulted in improved fracture strength of the molybdenum silicide. Such successes in improving molybdenum silicide could help the material join nickel aluminide alloys as strong candidates for a high-temperature materials hall of fame.



Weld macrostructure of an aluminum alloy and its associated hardness profile. *Electronic file enhanced by Allison Baldwin.*

System of Labs Approach to Welding, Direct Fabrication

ORNL, SNL, and INEEL are developing and testing hybrid techniques for welding steels and directly fabricating tools and dies.

In 1996 Al Narath, who then managed Lockheed Martin's Energy and Environment Sector, had a bright idea: Why not apply the unique expertise and capabilities of the sector's three DOE national laboratories to meeting critical national needs, such as improving industrial competitiveness? Why not focus the talents of groups from the three different labs on difficult, important problems through a "system of laboratories" approach? He proposed that such an approach would (1) speed the development of advanced technologies and their transfer to the commercial sector, (2) avoid duplication and competition among the laboratories while expanding their capabilities, and (3) make more efficient use of limited funding.

As a result of this System of Labs initiative, ORNL, Sandia National Laboratories (SNL), and Idaho National Engineering and Environmental Laboratory (INEEL) are working together on welding science and the direct fabrication of structural components using rapid manufacturing technology. The initial funding for these collaborations came through the Laboratory Directed Research and Development Program of each lab.

The welding collaboration (ORNL, Oak Ridge Y-12 Plant, SNL, and INEEL) has resulted in a successful proposal to DOE's Office of Industrial Technology on developing a process to combine laser welding and arc welding to weld steels for automotive applications. This proposal will bring $100,000 a year to each site for three years (DOE is supporting 70% of the program, and the steel industry is funding the remaining 30%).

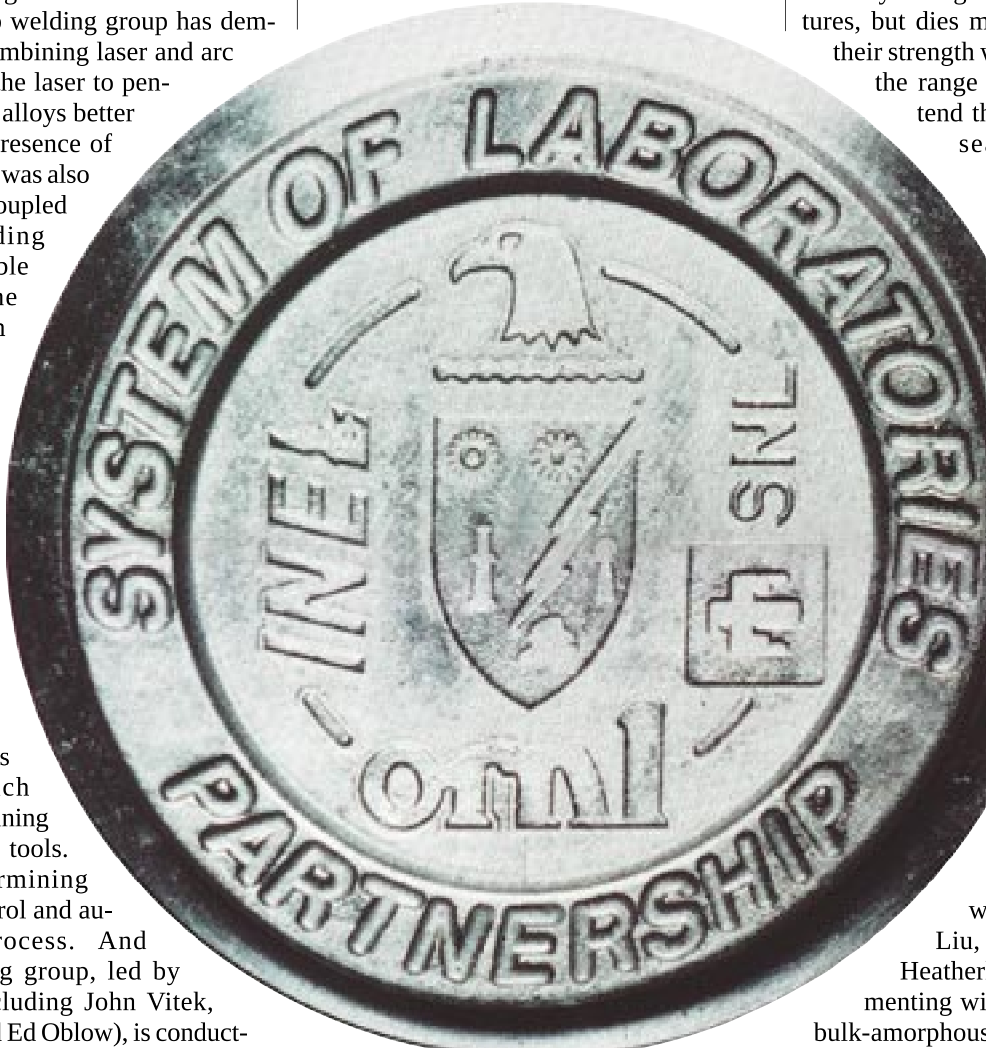
In the past year, the welding groups worked on developing a combined process for welding aluminum alloys, lightweight materials needed to make automobiles and aircraft operate more efficiently. They showed that it is possible to combine the processes to exploit the advantages and eliminate the weaknesses of each process.

Arc welding, in which a hot plasma produced by electrodes supplies the heat to melt and join two pieces of metal, has several advantages. It is commonly used, easy to control, and inexpensive. However, arc welding cannot be used at high speeds because it does not melt the metal enough to make a good joint. Laser welding can be used at high welding speeds with good penetration. However, it works well only when the pieces to be welded fit together neatly and when the surface is very clean. Also, laser welding does not penetrate aluminum alloys well because of poor coupling between the laser light and the material.

The three-lab welding group has demonstrated that combining laser and arc welding allows the laser to penetrate aluminum alloys better because of the presence of the arc plasma. It was also shown that the coupled laser-arc welding process is capable of achieving the desirable high welding speeds.

In the development of laser-assisted plasma arc welding and laser-assisted gas-metal arc welding, the three labs are playing distinct roles based on their strengths. SNL is developing each process by combining the two welding tools. INEEL is determining how best to control and automate each process. And ORNL's welding group, led by Stan David (including John Vitek, Suresh Babu, and Ed Oblow), is conducting properties measurements on welding samples and developing computer models (e.g., a neural network) to relate the samples' microstructures to their properties (e.g., hardness and ability to withstand loads). For example, the model can predict the shape of the weld based on parameters such as welding speed and power.

In research on direct fabrication, the goal is to produce a die (e.g., a mold for stamping out a product such as a beverage can) from a material in a single step instead of the usual multiple steps involving melting, casting, quenching, cutting, and machining, with various heat treatment steps in between. The idea is to form the die by depositing material using computer control. Researchers are comparing the performance of materials fabricated by conventional forming, spray forming (by INEEL), and laser-engineered net shape (LENS) technology (by SNL). The goal is to modify alloy compositions to improve performance of materials that could be used in the \$100-billion tool-and-die industry. Direct fabrication is expected to dramatically reduce the



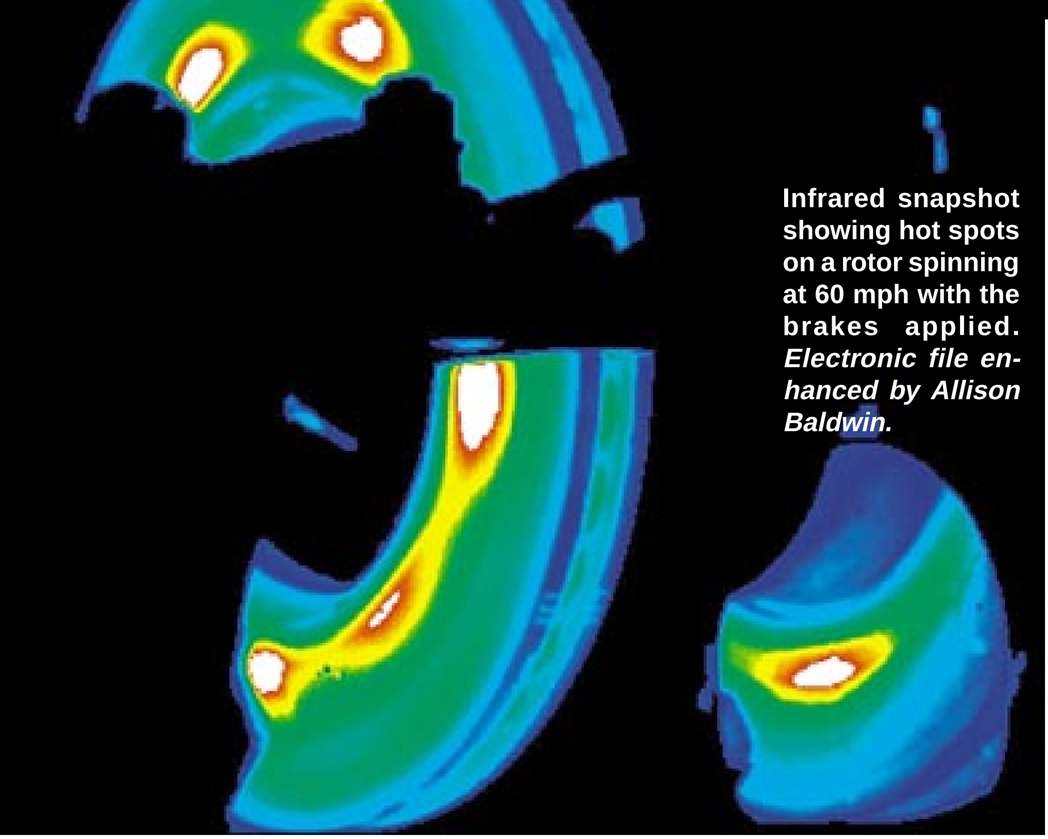
A metal piece showing logos of ORNL, INEEL, and SNL made by direct fabrication—spray forming by INEEL and LENS by SNL. *Electronic*

time and cost for developing complex dies and tools and to make a major impact on rapid prototyping.

In spray forming, metal from a molten ingot is sprayed and deposited layer by layer at a rate of 1000 pounds per hour. In LENS a light beam from a computer-controlled laser melts and deposits powder point by point to make any shape at a deposition rate of 2 pounds per hour. Although spray forming lays material down much faster than LENS, it cannot form certain desired shapes, such as tubes.

ORNL researchers led by Everett Bloom are searching for materials that could be deposited by a combined spray-forming–LENS process to produce any shape at greater speed. Studies show that dies made of carbide-strengthened H-13 steel are sufficiently strong and stable at low temperatures, but dies made of this material lose their strength when the temperature is in the range of 450 to 550°C. To extend the life of dies, ORNL researchers led by Phil Maziasz have modified the carbide composition of H-13 steel to make it more stable in dies used to make aluminum parts at temperatures up to 600–700°C. C. T. Liu's group has also developed a new nickel aluminide alloy for die—and tool—applications at temperatures up to 1000°C. Tests at SNL and INEEL are in progress to show that the new nickel aluminide alloy can be deposited by LENS- and spray-forming without technical difficulty. Liu, Dewey Easton, and Lee Heatherly have also been experimenting with making an iron-based-bulk-amorphous metallic glass, which is very hard and tough but low in friction and excellent in wear resistance. Such a shiny metallic glass would contain iron, titanium, and other elements. This material, which would withstand temperatures in the 400 to 500°C range, could be fabricated from a supercooled liquid, using less energy than is required by other forming methods.

These projects are only about a year old, but progress on both suggests that the System of Labs approach produces results that no one lab could achieve by itself. This new kind of national lab collaboration should help industry jump to the next level in economic competitiveness.



Infrared snapshot showing hot spots on a rotor spinning at 60 mph with the brakes applied. ***Electronic file enhanced by Allison Baldwin.***

Auto Disk Brake Hot Spots Seen By Infrared Camera

ORNL's modified infrared camera has imaged hot spots on auto disk brake rotors, which could lead to a better brake design and cut the auto industry's warranty costs.

You're driving fast when a deer crosses the road ahead. You slam on the brakes, avoiding a collision. That's the good news. The bad news is that the steering wheel shakes violently when you apply the brakes. Annoyed by the wobble, you take the car to the dealer and learn that the problem is "disk brake judder" and that the brake rotor may have to be refaced or replaced (at a cost as high as $200). Fortunately, the dealer will cover the cost because your car is under warranty, but that may not be true the next time you get brake judder. Because brake repairs cost the automobile industry and consumers billions of dollars, the U.S. industry is trying to determine the causes of brake judder and ways to prevent it.

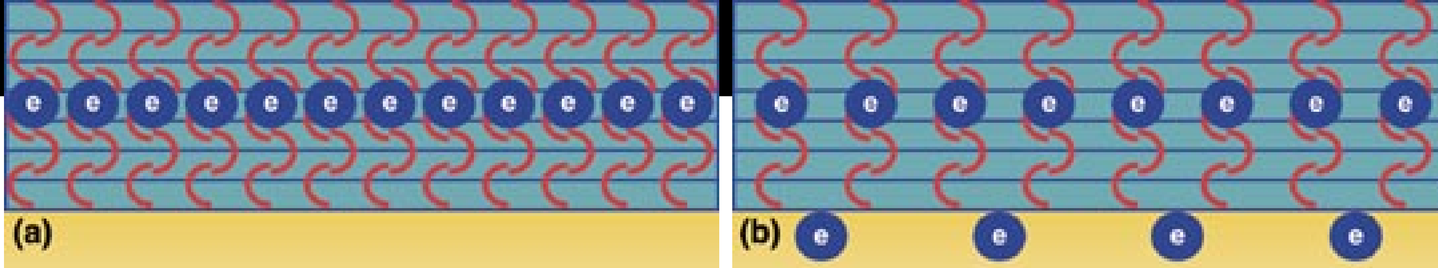
Using a high-speed, high-sensitivity digital infrared (IR) camera, ORNL researchers led by Ralph Dinwiddie have located and measured the temperature of brake disk "hot spots"—valuable information that may steer automakers toward a better brake design. The IR camera, obtained in 1996 from Amber, a Raytheon Company, has a temperature resolution of 0.015°C and takes 142 images per second (compared with a 0.2°C resolution and 30 images per second for a conventional IR camera). Through reverse fellowships and user projects with Ford Motor Company, General Motors Corporation–Delphi Chassis Systems, and Bosch Braking Systems, ORNL researchers have taken the IR camera to these companies' Michigan and Ohio sites for brake studies. But first they had to make the camera setup portable by configuring it to operate with a laptop computer. They also developed the interface circuitry to enable synchronized time-lapse thermography; thus, they can capture images of hot spots on a spinning brake rotor every three revolutions over a four-minute period.

A disk brake is a disk-shaped rotor that spins until pads rub against its surface when you depress the brake pedal, slowing or stopping the car. Using the IR camera, ORNL researchers were the first to image hot spots, or localized expansions, that develop in gray cast iron rotors when brakes are applied at high speeds. As the brakes heat up, areas of the rotor surface are raised, like turning an ordinary potato chip into a Pringle®. These raised areas drag more aggressively against the brake pads when pressed against the rotor, causing steering wheel vibrations.

By capturing multiple images of a spinning rotor, the infrared camera records temperature changes in hot spots that are observed to drift around the rotor. From this information, auto industry researchers have learned that the amount of friction (coefficient of friction) between the pads and rotor, their ability to conduct heat (thermal conductivity), and the amount they expand (thermal expansion) in response to heat cause distortions in the rotor at or above a "critical speed." This critical speed for the hot spots to develop is often below highway speed limits, so the auto industry would like to find ways to significantly increase the critical speed.

To achieve this goal and reduce the probability of brake judder, changes will have to be made in the design of the rotor and composition of the brake pads, which now are made of graphite, copper wires, brass fibers, kaline (clay), and even nut shells. ORNL's infrared camera is being used to determine whether design and composition changes are minimizing the evolution of hot spots. If the auto industry is successful in selecting the right design and materials, it could slow down an annoying drain on its profits.

This research is sponsored by the DOE's Office of Transportation Technologies as part of the High Temperature Materials Laboratory Programs. Funding to purchase the camera was provided by the Advanced Turbine Systems Program of DOE's Office of Industrial Technology to determine how well ceramic coatings on turbine blades hold up in a high-temperature environment.



Schematic representation of the "electronic growth" concept. In (a), as a metal (blue) is added onto a semiconductor substrate (yellow) layer by layer, the motion of the conduction electrons in the metal film is confined by the two vacuum-metal and metal-semiconductor interfaces, forming electronic standing waves (red). These waves resist being squeezed any further, helping to stabilize the film. In (b), some electrons leak into the semiconductor, weakening the stabilizing force. These two competing effects determine the critical thickness for smooth film growth. ***Drawing by Allison Baldwin.***

Metallic Thin Films and Magic Numbers

Theoretical studies at ORNL provide new understanding of the metal-semiconductor interface and of a different approach to growing smooth metal films on semiconductors.

For decades it has been known that certain nuclei are more stable than others and that certain atoms are inert while others are active. In the 1980s, physicists at the University of California at Berkeley discovered that, when atoms form clusters, certain clusters are also more stable than others. These systems are particularly stable when they each contain a "magic number" of constituent particles: protons and neutrons for the nuclei, electrons for the atoms, and atoms for the clusters. Now, an ORNL team is finding evidence for magic numbers in a new territory—the growth of metal films on semiconductor substrates.

Metals in contact with semiconductors are essential components in electronic devices ranging from small computers to smart cards. Because of the trend of device miniaturization, it is often desirable to form two-dimensional, atomically flat metal overlayers. Unfortunately, because of strain effects, most metal atoms deposited on a semiconductor surface naturally form three-dimensional clusters, leading to a rough film. Recently, a University of Texas group showed that an atomically flat silver film could be grown by depositing silver atoms on a gallium arsenide (GaAs) surface at 140 K and then annealing it to room temperature. The atomic flatness of the film was verified using a scanning tunneling microscope. The Texas study showed that smooth film growth could be achieved, but only above a critical thickness of seven layers of atoms (15 angstroms thick). The existence of such a critical thickness was unexpected, given commonly recognized growth mechanisms involving individual atomistic processes or strain effects.

How the critical thickness is attained was explained in 1997 by Zhenyu Zhang, a solid-state theorist at ORNL, in collaboration with the Texas group. Their theoretical work on deposition of metals on semiconductors has resulted in the formulation of a conceptually new mechanism for smooth film growth. The theory, which shows the importance of quantum effects in thin-film growth, can be explained by textbook-level quantum mechanics (particles in a box). When a metal film is thin, the moving conduction electrons within the film are confined in the film thickness direction—on one side by the vacuum and on the other by the metal-semiconductor interface. This "squeezing" of the electronic motion leads to quantized energy levels for the electrons, increasing the total energy of the system. However, because many more conduction electrons are in the metal than in the semiconductor, some electrons will spill from the film into the substrate, decreasing the system's energy. The competition between the two effects—quantum confinement and charge spilling—determines the observed critical thickness.

Within this "electronic growth" mechanism, Zhang and collaborators predicted that a critical thickness of a few atomic layers should also exist for the growth of two other noble metals (copper and gold) on GaAs and that only the first atomic layer of any alkali metal can be grown smoothly. For some other metals, smooth metal films can be formed only at certain magic numbers of atomic layers. Therefore, this theory promises to predict what amount of which elements should be deposited on which substrates at what temperatures to obtain the smoothest metal films.

In studying the transport properties of metal films, Zhang and his postdoctoral research associate Jun-Hyung Cho predicted an unexpected phenomenon related to depositing one antimony layer at a time on GaAs. If the film has one layer, it is insulating (electrically nonconducting), but if a second layer is added, the film becomes metallic (electrically conducting). Conventional wisdom says that adding another layer of metal to a metallic film can only make the thicker film more metallic. But Cho and others predict that with three layers of antimony, the film becomes insulating again and only when the film contains four or more layers of antimony will it maintain its metallic property. This prediction is being investigated experimentally by an ORNL surface physics group.

This theoretical work provides new understanding of the metal-semiconductor interface and of a different approach to growing smooth films. It also suggests that it may be possible to do quantum engineering of metallic overlayers down to the atomic scale, enabling the fabrication of perfect films needed for developing next-generation electronic devices.

The research was sponsored by ORNL's Laboratory Directed Research and Development Program and the U.S. National Science Foundation.

Physical Sciences and Neutron Science and Technology

ORNL has long been a leader in nuclear physics, atomic physics, and solid-state physics, as well as chemistry, in support of energy technologies. In 1997 the first experiment was performed at our unique Holifield Radioactive Ion Beam Facility (HRIBF). Our physicists refined HRIBF experiment stations, improved a proton source, and developed radioactive ion beams for studies of nuclear structure and nuclear astrophysics. In nuclear astrophysics research involving our Oak Ridge Electron Linear Accelerator, we collected and analyzed neutron capture data for use in computer models; the data are improving our understanding of the origin and nature of flecks of "red giant" stardust in meteorites. In the area of chemistry, we are developing a second-generation mass spectrometer for the U.S. Army to detect chemical and biological warfare agents. And some important findings have come out of our chemical studies to better understand why it's so difficult to convert low-rank coals to clean liquids.

Stemming directly from the Laboratory's original mission, ORNL's strengths in neutron-based science and technology include the design and operation of neutron sources (reactors and accelerators) and the use of neutrons in science and technology (neutron scattering, isotope production, neutron activation analysis, materials irradiation, and molecular structure determination). A more detailed understanding of magnetism and superconducting materials is one of our achievements using neutron scattering. ORNL's High Flux Isotope Reactor provides the world's highest thermal neutron flux, the only domestic source of heavy transuranic isotopes, and specialized neutron activation analysis for sensitive measurements of trace elements. Capabilities in this area support fundamental nuclear physics research, studies of material properties, nuclear materials management, development of materials for nuclear fusion and fission, isotope production for industrial and medical applications, and environmental protection.

First Experiment Performed at Unique Radioactive Ion Beam Facility

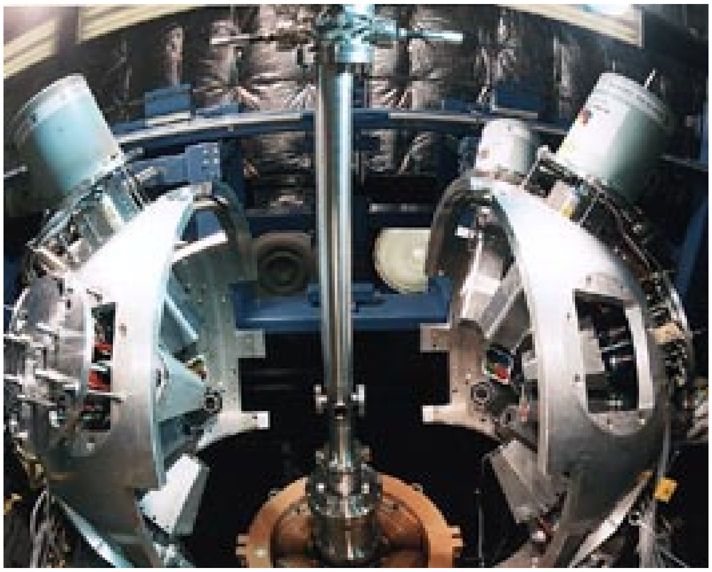
ORNL physicists and engineers refurbished and improved existing accelerators and designed and built a beam preparation system to provide a new and unique research capability—accelerated radioactive ion beams for research in nuclear structure and nuclear astrophysics.

Experiments under way at ORNL's new Holifield Radioactive Ion Beam Facility (HRIBF) will provide valuable data on the formation of heavy elements in stars and the peculiar structure of nuclei that have neutron and proton numbers far from those of stable nuclei that form most matter on earth. HRIBF, a unique tool for research in nuclear astrophysics and nuclear structure physics, began operation in March 1997, shortly after construction and commissioning of the facility were completed. The first experiment was run then at HRIBF by scientists from Yale University, Clark University, and Brookhaven National Laboratory.

HRIBF, which has been under construction since late 1992, is a part of the rapidly expanding new field of radioactive ion beam (RIB) research. Major projects are being developed in Europe and Japan, but, for the time being, HRIBF is unique in the range of radioactive species and beam energies it offers for research in nuclear structure physics and nuclear astrophysics.

A conventional nuclear physics facility accelerates beams of stable nuclei and directs them onto targets to generate nuclear reactions for further study. However, many of the most interesting questions in nuclear science can be answered only with beams of nuclei that are unstable, or radioactive. At HRIBF, unstable nuclei are produced in hot, thick targets by intense beams of protons, deuterons (proton-neutron combinations), or helium ions delivered from the Oak Ridge Isochronous Cyclotron (ORIC). These radioactive atoms are diffused out of the target, formed into an ion beam, purified by mass selection, and injected into ORNL's 25-million-volt (MV) tandem accelerator, which accelerates the beam to energies up to several hundred million electron volts. This high-energy beam is then directed to a target for physics experiments.

For the March 1997 nuclear-structure experiment, two radioactive ion beams were produced—arsenic-69 (^{69}As) and gallium-67 (^{67}Ga). Each beam was directed at a carbon target, which was used as a source of virtual photons to excite the low-lying states of the projectile nuclei. When the excited ^{69}As or ^{67}Ga nuclei returned to their lowest energy state, they gave off gamma rays, which were detected by a Yale instrument.



The target position gamma-ray detector array of the Recoil Mass Spectrometer, the flagship piece of new experimental equipment for HRIBF. ***Photograph by Lynn Freeny.***

During 1997, ORNL physicists and other staff conducted many stable beam experiments to commission and refine several million dollars' worth of new research equipment for physics studies. This equipment comprises the nuclear structure end station (Recoil Mass Spectrometer) and the nuclear astrophysics end station (Daresbury Recoil Separator). In one of these experiments, a new isotope of the element thulium (^{145}Tm) was identified. This isotope, which is very "proton-rich" (69 protons and 76 neutrons) for such a heavy nucleus, decays by a rare decay process, the emission of a proton from its ground state. The measured half-life of 3.5 microseconds for the ground state of ^{145}Tm makes it the shortest-lived proton emitter known.

ORNL staff accelerated three different radioactive ion beams (^{69}As, ^{70}As, ^{67}Ga) and developed low-energy, proton-rich beams of fluorine-17 and fluorine-18 (which have not yet been accelerated in the tandem) for use in 1998 for nuclear astrophysics experiments. They also are developing nickel-56 and copper-58 beams for nuclear structure experiments. Neutron-rich RIBs will also be produced by inducing fission in uranium and other heavy actinide targets. One neutron-rich RIB, tin-132 (^{132}Sn), is of great interest to nuclear structure experimenters because of its closed neutron and proton shells of 50 protons and 82 neutrons. The heaviest stable isotope of tin is ^{124}Sn, which has only 74 neutrons.

The development of HRIBF was a major technical achievement, carried out at very low cost. The RIB injector (target, ion source, mass selection, etc.) was designed and implemented from scratch. Two existing accelerators, the ORIC and the 25-MV tandem, have been adapted for radioactive ion beam production and acceleration. Finally, two state-of-the-art experimental stations were developed to support the very complex, difficult experiments that will be carried out at HRIBF in the years to come.

HRIBF is supported by DOE's Office of High Energy and Nuclear Physics, Division of Nuclear Physics.

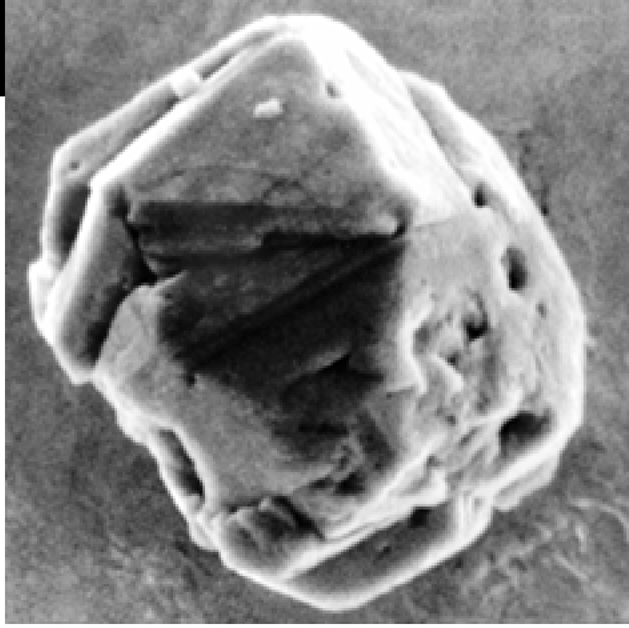
Stardust with Red Giant Fingerprints?

ORNL neutron capture data aid understanding of the origin and nature of stardust in meteorites.

Stardust—tiny particles from stars that rode to the earth on meteorites—is thought to contain the fingerprints of a red giant star. These fingerprints tell something about how elements were synthesized inside a very large, bright, low-mass star near our solar system around the time of its birth roughly 4.5 billion years ago. This red giant cast off its outer layers during recurrent flashes of violent helium burning before shrinking to a white dwarf, a whitish star that is very small, dense, and low in luminosity. Among the ashes churned out by the burning were microscopic grains of silicon carbide (SiC) whose existence could lead to new insights about the inner life of such stars, the origin of chemical elements and their isotopes, and the formation of our solar system.

The SiC grains appear to contain traces of the elements formed in the star by the "slow neutron capture process." In this so-called "s" process, heavy elements are synthesized (starting from iron "seed" nuclei produced by a previous generation of stars) through a chain of nuclear reactions involving the capture of neutrons by nuclei until a radioactive isotope is reached. At this point, beta decay (a process in which a neutron in the nucleus decays into an electron and a proton) transmutes the nucleus from one element to another. The "s" process, together with the "p" process and the "r" process (which are thought to occur in supernovae explosions), are responsible for the formation in stars of the elements between iron and uranium.

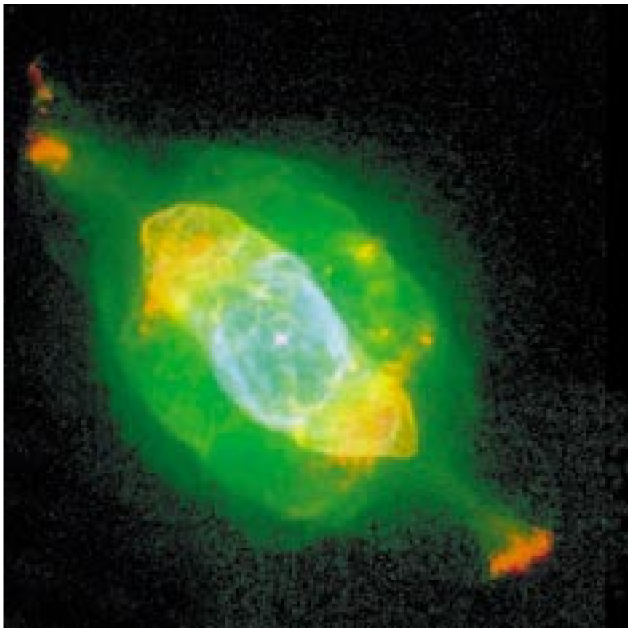
Since the 1970s, scientists at the University of Chicago and later Washington University in St. Louis have been measuring the pattern of abundances of trace elements and their isotopes captured in SiC grains found on the Murchison meteorite (which fell on Australia in 1969). The relative amounts of the various isotopes of several different elements determined from the analysis of the meteorite grains were found to be different from the patterns found in average solar system material. The hypothesis: the grains reflect the chemical and isotopic composition of a single star, but average solar system material is a mix from several different sources and processes.



Electron micrograph of a silicon carbide grain, probably from a red giant. It rode to the earth on a meteorite.

The precision of the analysis of the SiC grains has improved in the past few years because of the availability of more sensitive techniques. In the same period, a new computer model of nucleosynthesis processes in red giant stars has been developed at the University of Turin in Italy. The stellar model is being refined by its developers to predict accurately isotopic abundances in red giant stars by comparing its results with the meteorite data. To make its predictions, the red giant model must have the best possible neutron capture data, which are being supplied by researchers at Karlsruhe, Germany, and ORNL's Oak Ridge Electron Linear Accelerator (ORELA).

The new red giant model predicts that the temperature at which the s process produces elements in stars is around 70 to 90 million degrees, a factor of five lower than the originally calculated 350 million degrees. ORELA is ideally suited to provide precise determinations of the neutron capture rates at these lower temperatures.



Red giants form planetary nebulae (like the one in the above image captured by the Hubble Space Telescope) in which silicon carbide dust grains can be found. *Electronic file enhanced by Allison Baldwin.*

Using ORELA (whose useful neutron energies range from 0.02 electron volts to 40 million electron volts), Klaus Guber, Paul Koehler, and their colleagues for the first time experimentally determined the neutron capture reaction rates for isotopes of neodymium (Nd) at the new low temperature needed by the red giant model. When their data were used, precise agreement was obtained between the red giant model predictions and the Nd isotope ratios determined from measurements on SiC grains from the Murchison meteorite. However, more recent measurements at ORELA on barium isotopes have revealed a substantial discrepancy between the red giant model and the meteorite data. It is hoped that the discrepancy will lead to new insights into the origin and nature of this stardust. ORNL researchers are doing additional experiments at ORELA to provide more data with which to constrain and improve the red giant model.

The research is supported by DOE's Office of Energy Research, Office of Basic Energy Sciences, Division of Nuclear Physics.

Marcus Wise (left), Steve Lammert, and Cyril Thompson show the analyzer and its electronics in a testbed for evaluating systems of the new chemical-biological mass spectrometer. They are part of a 50-person ORNL team developing the instrument for the Army. *Photograph by Tom Cerniglio.*

Warfare Agent Mass Spectrometer Being Built at ORNL

ORNL is developing a second-generation mass spectrometer for the Army to detect chemical and biological warfare agents.

Seven years ago, during the Persian Gulf War, the U.S.-led multinational coalition that ousted Iraqi military forces from Kuwait used various detectors to try to determine if coalition forces were being exposed to Iraqi chemical warfare agents. Many false alarms were sounded because the chemically complex background of fumes from oil well fires, fuels, and lubricants, as well as exhausts from weapons and engines, confounded the detectors. As the health problems experienced by some veterans illustrate, the instrumentation used to detect and identify chemical warfare agents in the field has not been particularly reliable. Detection of biological warfare agents, such as toxins, viruses, and pathogenic bacteria, is even more difficult.

Because of its world-class expertise in mass spectrometry, ORNL was contracted by the U.S. Army Chemical and Biological Defense Command to design and construct prototypes and preproduction models of the next series (the Block II) of the chemical-biological mass spectrometer (CBMS) for rapid field detection and identification of chemical and biological warfare agents. This four-year, $32-million program includes 50 researchers from five ORNL divisions, three academic and commercial subcontractors, and four Department of Defense facilities or laboratories. Orbital Sciences Corporation will help design the CBMS to make it economically produceable in the commercial sector. Spin-off civilian uses of the CBMS technology may include rapid bacterial detection and identification in the health care and food processing industries, as well as environmental pollution mapping and civil defense.

The Army called for the next-series instrument to be smaller, lighter, faster, less expensive, more sensitive, more rugged, and more easily maintainable. It also should be able to detect and distinguish among a wider variety of airborne chemicals and microorganisms, as well as chemicals on the ground, than does current instrumentation. The Block II CBMS will consist of five modules; the total package will be about the size of a desktop computer and monitor. The heart of the Block II CBMS is an ion trap mass spectrometer similar to the ORNL instrument successfully deployed for field analytical measurements of hazardous chemical pollutants.

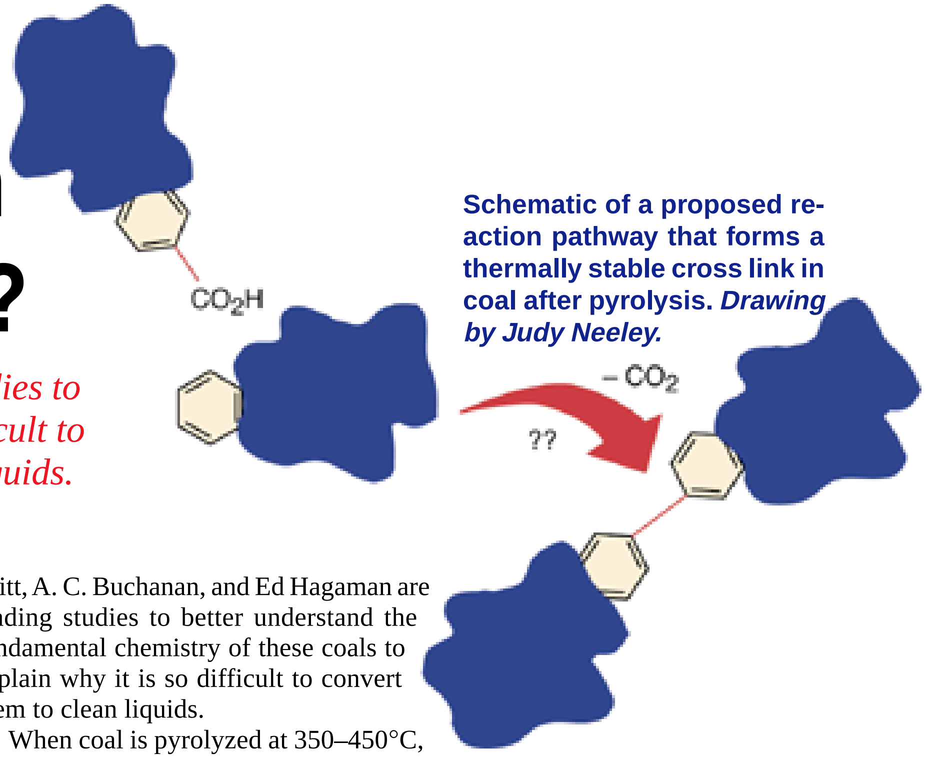
The CBMS will sample air and collect, classify, and concentrate micron-sized particles of biological warfare agents such as anthrax spores or bacterial toxins. The biomarkers in the biological agents are released and introduced into the ion trap by a combination of pyrolysis and in situ methylation. In the spectrometer, the biomarker molecules are ionized, selectively accumulated, separated in an electric field, and detected. Sophisticated identification algorithms are required to detect and identify biological agents present in a background that may include naturally occurring microorganisms, pollen, mold, and fungus. Chemical warfare agents (e.g., the nerve agent VX or blister agent HD) are much more easily detected and identified in ground surface and air samples by their known, characteristic ions.

The CBMS team's researchers have introduced several innovations to improve the instrument to meet the Army's goals. In addition to the instrumental innovations by ORNL analytical chemists, ORNL computer scientists are developing data acquisition, manipulation, and display systems. Our electrical engineers are designing the circuitry to include state-of-the-art components that can perform advanced functions and yet maintain physical ruggedness and radiation tolerance. Facilities are being established at ORNL for testing the CBMS units with very small quantities of the targeted agents before they are delivered to the Army for acceptance tests.

The final product will provide vastly improved protection to our troops. It should not sound any false alarms, but it is hoped there will be no need for real ones.

Can Fuels Be Made from Inferior Coals?

ORNL is conducting chemical studies to better understand why it is so difficult to convert low-rank coals to clean liquids.



Schematic of a proposed reaction pathway that forms a thermally stable cross link in coal after pyrolysis. *Drawing by Judy Neeley.*

During the oil embargo of the 1970s, the temporary shortage of imported oil forced Americans to wait in long lines to fill their cars with gasoline. One proposal for bypassing unreliable oil sources was to produce an alternative fuel from coal. The idea was to pulverize coal, mix it with a solvent that donates hydrogen to it (because coal is hydrogen poor compared with oil), heat it in the presence of hydrogen to break its chemical bonds in a process called pyrolysis, and refine the resulting liquid for use as transportation fuel for vehicles. Coal liquefaction pilot plants were built in the United States, but they eventually closed because climbing oil prices later fell, making coal liquids uncompetitive.

But basic research in support of coal liquefaction is still alive at ORNL and a few other institutions. In fact, ORNL organic chemists have broadened their research effort to study oil shales and renewable resources such as lignin from waste wood. Their goal is to pin down the relationship between molecular structure and chemical reactivity in organic energy resources. Coal is particularly challenging because it is an amorphous, insoluble hodgepodge of organic materials and inorganic minerals with no repeating units as are present in crystals and in polymers.

U.S. reserves of high-carbon, high-energy coals—anthracite and bituminous coals—are quickly becoming depleted, so U.S. electric utilities and other industries are relying more on our cheap, abundant supplies of low-rank coal from surface mines in the western United States. These subbituminous and lignite coals are lower in carbon and hydrogen content but higher in oxygen than bituminous coals, making low-rank coals harder to liquefy than the high-carbon coals. ORNL chemists Phil Britt, A. C. Buchanan, and Ed Hagaman are leading studies to better understand the fundamental chemistry of these coals to explain why it is so difficult to convert them to clean liquids.

When coal is pyrolyzed at 350–450°C, the quality and yield of the products formed depend on the extent of chemical bond breakage to make small molecules, the donation of hydrogen to coal to make petroleum-like liquids, mass transport, and cross linking—the retrogressive process by which smaller molecules form larger molecules. Of these processes, cross linking is least understood. Therefore, ORNL chemists have focused their research on oxygen-containing heteroatom compounds (e.g., carboxylic acid, phenols, and ethers) which are thought to be responsible for the formation of thermally stable cross links in low-rank coals (requiring temperatures greater than 600°C to break).

In the mid-1980s scientists from Lehigh University, Brown University, and Advanced Fuel Research pyrolyzed samples of low-rank coal and analyzed the evolved gases, such as carbon dioxide, carbon monoxide, methane, and water vapor. For low-rank coals, cross-linking occurred simultaneously with carbon dioxide evolution. Later research results suggested that carbon dioxide was produced by pyrolysis of aromatic carboxylic acids [carbon atom linked to an oxygen atom and a hydroxyl group (OH), represented as CO_2H].

Applying the tools of organic chemistry to this problem, ORNL researchers followed reactions of their model coal compounds and a polymer analog they had synthesized and related their observations of the pyrolysis chemistry back to coal. They looked for different reaction pathways involving aromatic carboxylic acid, whose existence and abundance in coal was determined by Hagaman using solid-state nuclear magnetic resonance spectroscopy. Their studies showed that thermal decomposition of aromatic carboxylic acids produced carbon dioxide but was not responsible for the formation of the thermally stable cross links, suggesting that computer models for the pyrolysis and liquefaction of low-rank coals should be changed.

So, what was the source of the thermally stable cross links? The ORNL researchers' recent studies suggest that, during pyrolysis, two acids combine to form an anhydride cross link, and a molecule of water is released from the coal. The anhydride undergoes further reactions to form a thermally stable cross link. The chemists further suggested that coal structure researchers should look for evidence of anhydrides, and that the chemistry of coal liquefaction could be altered to stop anhydride formation, perhaps by running the process with water present.

All these findings could become valuable if the price of oil soars and coal liquids become competitive. It could happen, given the political instability of the oil-producing countries, and the first sign may be an unusually long line at the gas pumps.

The research was sponsored by DOE's Office of Energy Research, Office of Basic Energy Sciences, Division of Chemical Sciences.

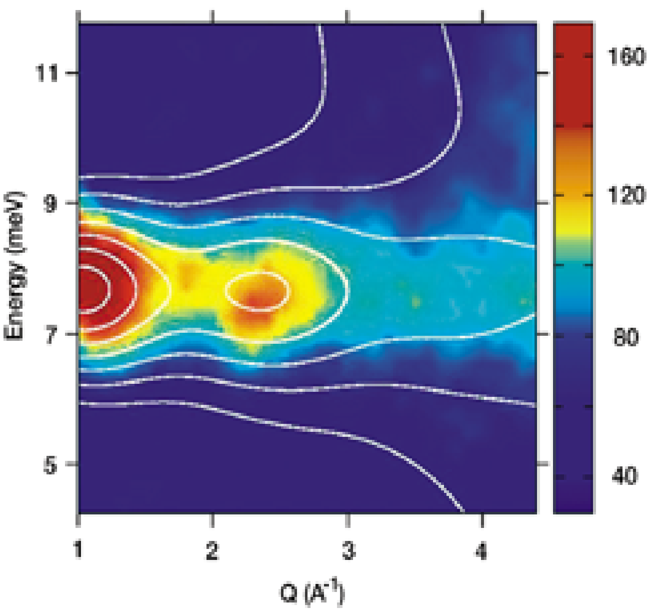
Quantum Leaps in Understanding Quantum Magnetism

ORNL neutron-scattering studies show that magnetic interactions in some magnetic chain materials are very different from what was previously believed.

When we hold a horseshoe magnet, we think of magnetism in three dimensions. Some scientists, however, view magnetism in lower dimensions. In fact, understanding lower-dimensional magnetism may lead to the design of improved superconducting materials with higher transition temperatures. In the high-temperature superconductor yttrium-barium-copper oxide (YBCO), scientists focus on copper, the material's only atom that has significant magnetic properties. Copper atoms exist in YBCO in a one-atom-thick plane (two dimensions) and in long chains (one dimension). Similar structures that have planes or chains containing magnetic atoms are found in many materials.

Physicists refer to the microscopic magnet of an individual atom as the "spin." Spins respond to one another by a mechanism known as a quantum mechanical exchange interaction. Isolated chains of magnetic atoms are referred to as spin chains. Two or more parallel spin chains together form structures known as spin ladders, which actually have a spatial dimension between one and two, which is especially interesting theoretically. Researchers in quantum magnetism are eagerly seeking to discover spin ladders and chains in materials that might lead to new families of high-temperature superconductors.

Scientists had suggested that the best example of a spin ladder found in nature was a phosphate salt containing magnetic vanadium ions, called VOPO [$(VO)_2P_2O_7$]. This idea was widely accepted until neutron-scattering studies of this material by ORNL's Stephen Nagler and colleagues showed that VOPO is really a different type of magnetic beast called an alternating spin chain. Alternating chains and ladders do have some things in common: Both can be visualized as structures composed of interacting "dimer" building blocks, which are pairs of interacting spins. In addition, both have unusual "quantum spin gaps" such as are found in many of the most interesting materials currently studied by solid-state physicists.



Neutron-scattering pattern from a VODPO. White lines are theoretical contours for spin dimer model. ***Digital image enhanced by Allison Baldwin.***

To carry out neutron-scattering experiments at ORNL's High-Flux Isotope Reactor, the group used single crystals of VOPO grown by ORNL's Brian Sales. Andrew Garrett, a graduate student of Nagler's from the University of Florida, assembled an array of roughly 200 millimeter-sized VOPO crystals to make the neutron-scattering studies possible. The other members of the team are Alan Tennant, a postdoctoral researcher who recently came to ORNL from Oxford University's Clarendon Laboratory, and theoretical physicist Ted Barnes.

The single-crystal studies allowed the researchers to determine the spectrum of elementary quantum magnetic excitations (magnons) in VOPO, giving definitive proof of the alternating spin chain model. Nagler and associates also studied isolated vanadium spin dimers in a related material called VODPO. (The sample was provided by C.C. Torardi of DuPont). Here the ORNL studies found yet another surprise: The basic V-V dimer building block had been misidentified. The strong magnetic interaction was not between the closest pair of neighboring vanadium atoms as had been thought, but rather it was between a more widely separated V-V pair with a bridging phosphate (PO_4) group mediating the pair's magnetic interaction.

A third surprise from these studies was the discovery of a new kind of magnetic excitation in the VOPO alternating chains. Instead of seeing one peak from the neutron scattering, researchers saw two peaks. The unexpected peak may arise from a two-magnon bound state. Ted Barnes, who appeared on CNN after predicting the existence of the exotic meson which was detected experimentally in 1997 by DOE's Brookhaven National Laboratory, thinks that bound magnons will be found in magnetic spin ladders as well as alternating chains. Nagler says that the spin characteristics of free and bound magnons make them mathematically similar to mesons. In a quantum spin chain each magnon is really composed of two different quantum excitations called "spinons." Thus a two-magnon bound state has four spinons.

Similarly, mesons are composed of two quarks, and particle physicists hypothesize the existence of a mesonic molecule composed of four quarks (a proton and neutron are each formed from three quarks). Pending the outcome of this research ORNL may be able to claim discovery of an exotic magnetic excitation, which to some scientists, is far more interesting than an ordinary horseshoe magnet.

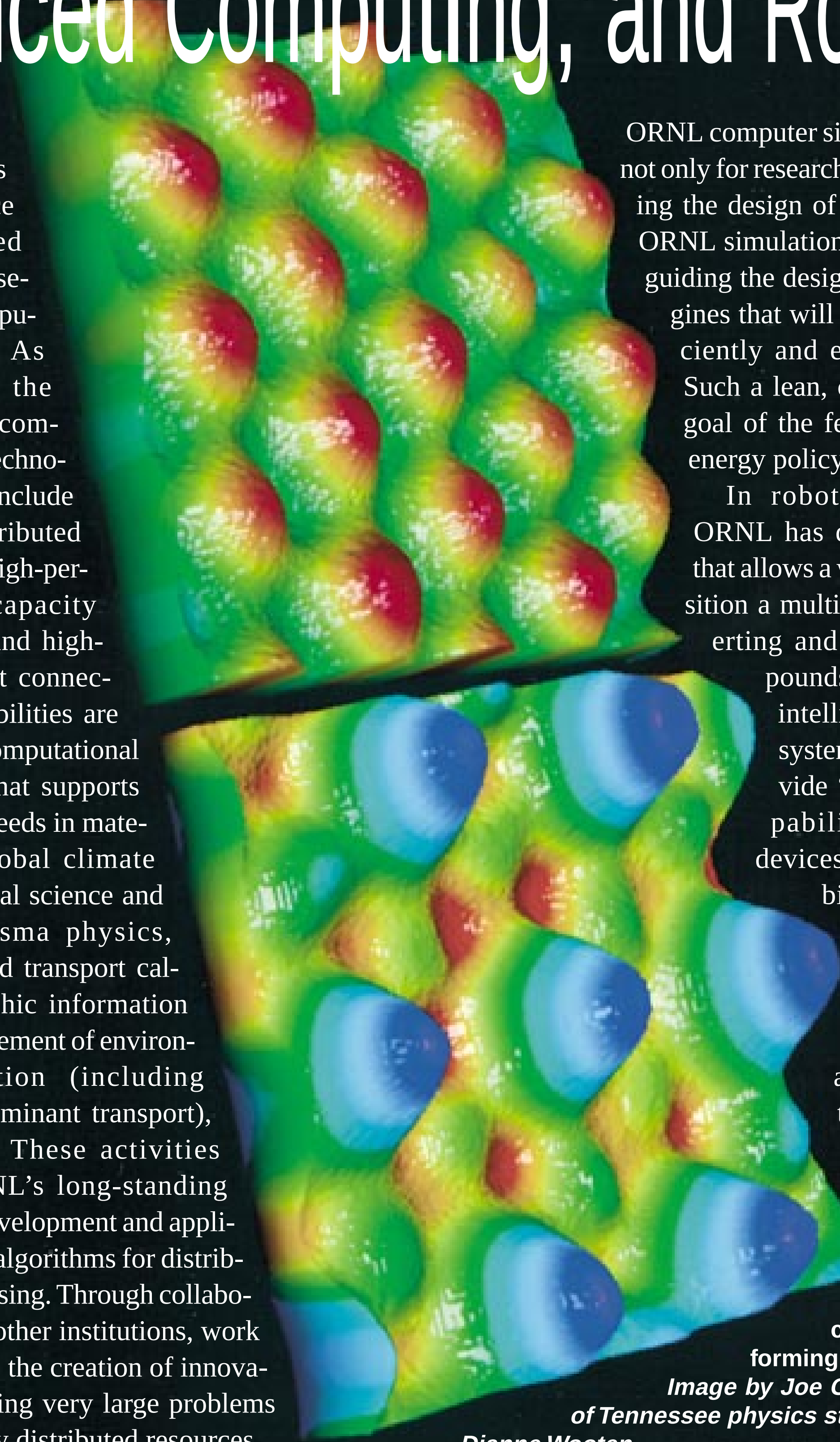
The research was sponsored by DOE's Office of Energy Research, Office of Basic Energy Sciences.

Computational Science, Advanced Computing, and Robotics

ORNL is one of the world's leaders in high-performance computing, related technologies, and selected areas of computational science. As home to one of the world's foremost computing centers, its technological resources include Intel Paragon distributed memory systems; high-performance, high-capacity storage systems; and high-bandwidth Internet connections. ORNL capabilities are integrated into a computational science program that supports national research needs in materials science, global climate simulation, chemical science and engineering, plasma physics, nuclear physics and transport calculations, geographic information systems, the management of environmental information (including groundwater contaminant transport), and informatics. These activities complement ORNL's long-standing leadership in the development and application of tools and algorithms for distributed parallel processing. Through collaborative efforts with other institutions, work in this area leads to the creation of innovative means of solving very large problems with geographically distributed resources.

ORNL computer simulations are useful not only for research but also for improving the design of industrial products. ORNL simulations of combustion are guiding the design of automotive engines that will burn fuel more efficiently and emit less pollution. Such a lean, clean car is a major goal of the federal government's energy policy.

In robotics development, ORNL has developed a device that allows a worker to lift and position a multi-ton payload by exerting and feeling just a few pounds of force. ORNL's intelligent transportation systems data bus will provide "plug and play" capability for electronic devices added to automobiles. The in-vehicle information system will manage "electronic traffic" within a car to avoid driver distraction.



ORNL's computer visualization capabilities enhanced this image of a charge density wave forming on a crystal surface. ***Image by Joe Carpinelli (University of Tennessee physics student) enhanced by Dianne Wooten.***

Accelerator, Code Yield Needed Data for Nuclear Safety

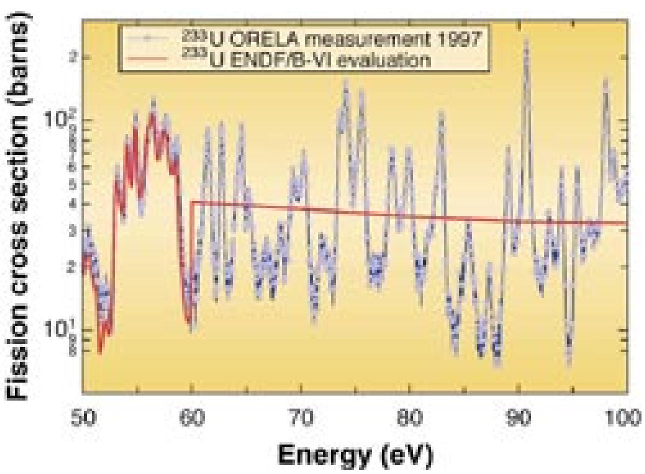
The Oak Ridge Electron Linear Accelerator and the ORNL computer code SAMMY provide the nuclear data necessary for reliable nuclear criticality safety studies.

Across the DOE complex, tons of nuclear materials have been warehoused for decades. Sometimes they are moved either within or between facilities. When masses of nuclear materials are collected this way, there is a potential for criticality, a condition that could accelerate into a radiation-releasing nuclear chain reaction.

Nuclear materials in close proximity react under certain conditions to produce neutrons through fission. A neutron-absorbing substance is arranged among stored nuclear materials to control reactivity. However, if the materials are not stored in proper configurations, they may produce more neutrons than can be absorbed. If neutron production and absorption become equal, a critical mass is reached. If production exceeds absorption, an uncontrolled chain reaction can ensue. To avoid a critical mass, the people handling nuclear materials need precise information about how much neutron multiplication will occur if specific masses are placed at particular distances from each other in a certain pattern. Nuclear engineers who address these issues must analyze all possible scenarios that might lead to criticality safety concerns, and nuclear data play a crucial role in their analyses.

Because of deficiencies in the data available for criticality safety studies, the Defense Nuclear Facilities Safety Board (DNFSB) asked ORNL for help. The DNFSB seeks to maintain U.S. capability for ensuring that nuclear materials being stored and transported are kept economically in subcritical arrangements. ORNL researchers, led by Bob Roussin and Luiz Leal, are using the Laboratory's Oak Ridge Electron Linear Accelerator (ORELA) and the ORNL computer code SAMMY to generate the needed data.

DOE installations store nuclear materials in configurations such that the neutrons produced cover the energy spectrum from slow to fast. In the past, nuclear data measurement and evaluation placed little emphasis on the intermediate energy range, which can be extremely important in nuclear criticality safety calculations. Consequently, existing data in the intermediate energy range are likely to be inadequate to provide results within the desired criticality safety margin. This lack of adequate data results in overly conservative and expensive shielding, transportation, and storage systems.



The impact of ORELA's capability to produce high-resolution neutron cross-section data can be seen in these fission cross-section measurements for uranium-233 (^{233}U), shown as circles. The heavy line shows the current ^{233}U representation in the Evaluated Nuclear Data File. Above 60 electron volts (eV), the detail in the cross-section data is clearly missing in existing files.

ORELA is an intense neutron source for measuring the probability (cross section) that any neutron will interact with or be absorbed by a particular atomic nucleus. ORELA is a unique tool for cross-section measurements. It produces neutrons in nanosecond-wide bursts, each of which contains neutrons with energies ranging from 10^{-3} to 10^8 electron volts. Precise measurements can be made because of ORELA's long flight path—up to 200 meters; the longer the neutron flight path, the greater the spread between the peaks and valleys of the cross sections and thus in the detail that can be gleaned. ORELA is the best U.S. source of high-resolution data in every neutron energy range, including the one of importance to the criticality safety program.

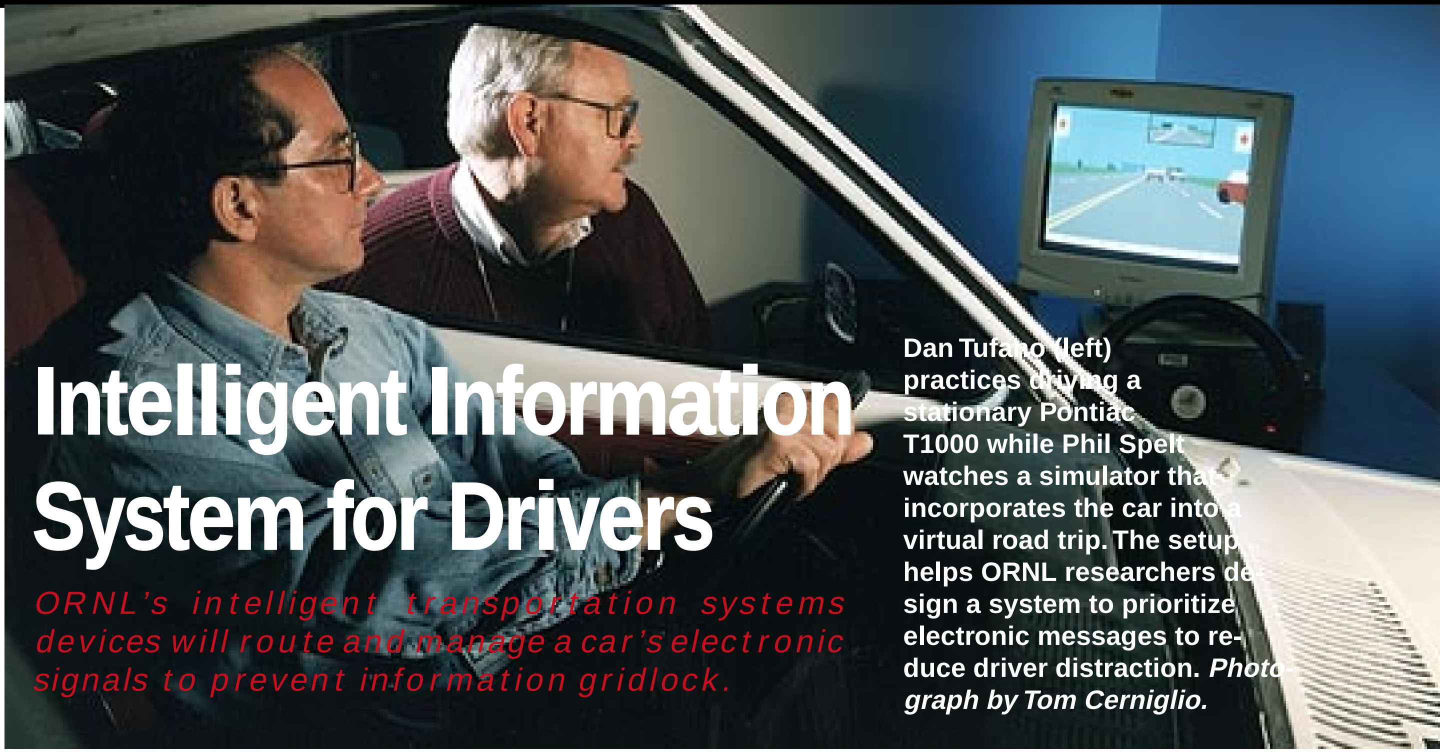
Because a vast amount of data is produced during an experiment, it is impossible to use the data directly to analyze and design a nuclear system. To make the measured data available in a form suitable for applications in nuclear technology, a procedure called nuclear data evaluation is used.

ORNL's computer code SAMMY, developed by Nancy Larson, is the best tool for evaluating neutron cross-section resonance data in the intermediate energy range. SAMMY provides uncertainties and correlations among data points (parameters) as a by-product of the evaluation process. These features play an important role in establishing uncertainty limits in analyses of nuclear criticality safety.

Evaluations using SAMMY are included in the national Evaluated Nuclear Data File and made available to the scientific community. The data are further processed into forms suitable for input to modeling codes such as KENO, MCNP, and VIM, which perform the actual criticality safety calculations for a given configuration of nuclear materials. The results allow nuclear engineers to infer how much absorber is needed in a given storage situation, how close the nuclear materials can be to each other, and how they can be arranged most economically to prevent criticality.

Using the unique capabilities of ORELA and SAMMY, nuclear analysts can ensure that cold war legacy materials are managed so that they remain a subcritical matter.

The project is funded by DOE's Environmental Management Program.



Intelligent Information System for Drivers

ORNL's intelligent transportation systems devices will route and manage a car's electronic signals to prevent information gridlock.

Dan Tufano (left) practices driving a stationary Pontiac T1000 while Phil Spelt watches a simulator that incorporates the car into a virtual road trip. The setup helps ORNL researchers design a system to prioritize electronic messages to reduce driver distraction. *Photograph by Tom Cerniglio.*

As you drive up I-75 to a meeting, several electronic signals bombard your car's computer network simultaneously: the navigation system reminds you to get off at the next exit, the collision avoidance system warns you about the car in your right-hand blind spot, your pager gets a message that the meeting room has been changed, and your cellular phone receives a call from home.

Now, which one of those signals would you like to receive first? If you get the exit notice before the collision-avoidance warning, or if you have to sort out all those messages at once, your automatic security system might soon be dialing 911 for you.

Every modern automobile relies on an onboard computer network. Considering the increasing numbers of devices that feed into the network, accommodating the electronic traffic and managing it to avoid signal gridlock are major concerns of automobile safety experts. To address these concerns, ORNL is helping to develop the intelligent transportation system (ITS) data bus (IDB), a data-routing system, and the in-vehicle information system (IVIS), an onboard information manager.

Automakers do not use a single standard for automobile data buses, channels along which data travel electronically. Because any electronic device added to a vehicle must be compatible with the data bus, the lack of a standard bus makes it necessary to build different versions of a product for various makes of cars. The IDB will provide "plug and play" capability for such devices, says ORNL developer Phil Spelt. Built according to a Society of Automotive Engineers standard, the IDB will plug into any vehicle's main data bus through a "gateway controller" that controls the data flow between the two buses. Add-on devices will then plug into the IDB. Having a single standard interface will allow device makers to design products that can plug into the data bus in any vehicle. In addition, many essential vehicle systems use the main bus to send data that must be shielded from interference from add-on devices; the IDB, by regulating data flow between the main bus and add-ons, will provide that protection.

The IVIS will function as an information manager to filter and prioritize information from the multiple devices that use the IDB. As experience with car phones has shown, drivers distracted by electronic gadgets are more likely to have accidents. As the number and variety of these products grow, so will the distraction, unless they can be prevented from competing for the driver's attention. The IVIS will monitor incoming signals to electronic devices, set priorities, and queue them for the driver's attention: this message about an accident is more important than the radio; this page can wait until you've seen the warning from the oil pump.

ORNL's IVIS project researchers have been asked by the ITS Data Bus Committee, which oversees IDB development, to help design testing protocols for electronic devices and conduct bench-level tests of the prototype IDB. In addition, several private companies have asked ORNL to help implement a prototype IDB within a vehicle. Chrysler and General Motors will donate a new vehicle for the project, and the prototype will be tested in the IVIS laboratory. ORNL is developing software to test the interfaces between the prototype IDB and devices plugged into it. Companies manufacturing electronic devices for autos will use the test results to improve the products.

ORNL also is developing the underlying logic for the software that will control the IVIS. To provide data for programming the IVIS, Spelt's team will place subjects inside a vehicle to "drive" in a simulated driving environment with projected scenes and sounds. Their responses to the driving environment, including signals from electronic devices, will be monitored and the data will be used in establishing the prioritization scheme.

The prototype in-vehicle IDB (which probably will include a rudimentary IVIS) is expected to be tested at automobile and trade shows around the country during 1998 and 1999. The IDB and the IVIS may be available commercially by 2005 to help drivers avert information gridlock.

Development of the IVIS was supported by the Federal Highway Administration, Information and Behavioral Systems Division. Funding for the IDB came from the Society of Automotive Engineers.

Computer Models Aim for Lean, Clean Engine Combustion

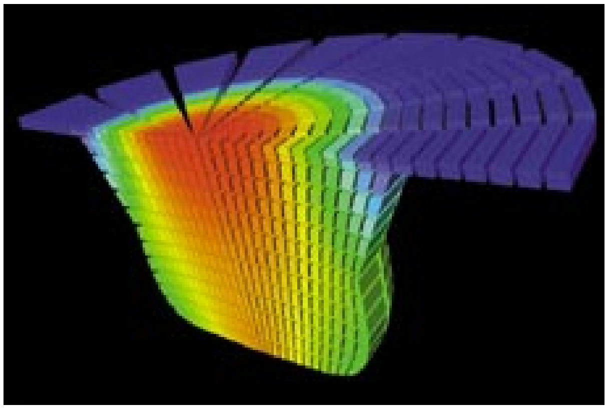
ORNL's model of spark energies is guiding the design of gas engines that will use less fuel and emit less pollution.

Many lean, clean cars of the future will have spark-ignited engines like the gasoline engines of today, but they may run on other fuels, such as natural gas. The reasons: Natural gas burns cleaner than gasoline and the United States has an abundant supply of natural gas. Lean-burn engines offer higher efficiency than conventional engines. Lean-burn natural gas engines would run more efficiently, reduce U.S. dependence on foreign oil, and emit less carbon dioxide, slowing the buildup of greenhouse gases in the atmosphere.

In such an engine, as each piston glides toward the top of a cylinder, it compresses the mixture of air and natural gas. Then a spark plug ignites the fuel-air mixture. An electrical current crossing the gap between the plug's electrodes at a voltage of 10 to 20 kilovolts ignites the gas in the gap. The combustion of the fuel-air mixture drives the piston, creating useful work at the flywheel.

The trick is to design natural gas engines and spark plugs to walk a fine line. If the deposited spark energy causes too hot a blast (2600 K), the engine will make the most efficient use of the fuel, but it will produce more nitrogen oxides—pollutants that contribute to the formation of acid rain and smog. Also, if the heat is too intense, it will rapidly erode the spark plugs, widening the gap between the electrodes and requiring a larger voltage to produce the needed ignition energy (some spark plugs last only about 200 hours because of erosion). If the spark plug voltage is too low, misfires result and the amounts of deposited energy are so low that much of the fuel remains unburned. The challenge is to design engine spark plugs to deposit energy in an amount high enough to achieve uniform combustion yet low enough to reduce emissions and spark-plug erosion.

Engine manufacturers such as Cummins Engine and General Motors are working to improve the designs of advanced engines, and ORNL is collaborating with them through cooperative research and development agreements by applying its expertise in computer simulation, spark stabilization, and engine diagnostics techniques. Using a suite of computational analysis tools, ORNL researchers led by Osman Yaşar, Jeff Armfield, and Isidors Sauers have developed a new spark ignition model and integrated it into the KIVA-3 engine combustion model. The model is being applied to newly designed Cummins Engine natural-gas (NG) and General Motors spark-ignited direct-injection engines that are being developed. This new spark ignition model provides the most detailed computation yet of the spark ignition process. When combined with ORNL's massively parallel version of the KIVA-3 engine combustion model, this new capability puts ORNL in a unique position in industry's eyes because of the ability to perform simulations of nanosecond-timescale physics and many-million-mesh-points spatial refinement of mathematical accuracy.



Temperature profile of combustion (the red part is the hottest) seen in a cross section of a spark-ignited internal combustion engine cylinder whose piston is near the top. *Digital image enhanced by Allison Baldwin.*

Conventional models assume a constant, uniform deposition of spark energy, but the ORNL model shows that energy deposition is nonuniform and that temperatures throughout the spark gap area vary with location and time after ignition. The model correlates spark input parameters (e.g., discharge current, breakdown voltage values, spark duration) with engine output (i.e., efficiency of energy use and emission levels). The ORNL simulation results are expected to have an impact on the design of combustion engines by defining lean fuel limits and optimum spark energies that will result in lower fuel consumption, more efficient burning of the fuel, and reduced emissions.

ORNL's scalable combustion model is also being improved with the addition of a new radiation transport submodel that will be used to analyze coal combustion for utility boilers. ORNL and McDermott Technologies, Inc. (formerly known as Babcock & Wilcox) have an active collaboration to improve boiler designs through simulations on ORNL's massively parallel computers. In this type of combustion, 80% of the heat from the coal is transferred by radiation. Because the radiation changes much faster than the background flow motion (nanoseconds vs microseconds), it is fortunate that the ORNL model can simulate these changing dynamics by showing in detail the different length scales and time scales involved in physical phenomena.

ORNL's developments in spark ignition and radiation transport simulations not only open opportunities for the design of improved engines and boilers but also open avenues for basic research in plasma physics, computational science, and mathematics. The ORNL models may help engine designers think lean while providing meat for physicists, mathematicians, and computational scientists.

The research is sponsored by DOE's Office of Computational and Technology Research, Division of Mathematical, Information, and Computational Sciences; by DOE's Office of Energy Efficiency and Renewable Energy; and by matching funds from Cummins Engine, General Motors, and McDermott Technologies.

ORNL Device Gives Big Lift to Operators with Heavy Loads

ORNL has developed a "human amplification" device that allows a worker to lift and position a multi-ton payload by exerting and feeling just a few pounds of force.

When Sigourney Weaver straps on a robot suit that turns her into a gigantic kickboxer in the movie *Alien II*, it's all make-believe. But an ORNL-developed system based on the same concept works in the real world.

The concept is the engineers' dream of human amplification. A machine gives you the power to lift and handle multi-ton objects using only your hand's force. Because you can feel the forces operating on the payload, you can precisely and safely control and manipulate the load.

In a demonstration of the Advanced Telerobotics Technology Demonstrator (ATTD), an implementation of ORNL's human amplification technology, a single person deftly picked up a 2500-lb weapon and hooked it onto small holding brackets under the wing of a plane. The task usually requires several people; a crane and rigging equipment; and quite a bit of time to rig the weapons, position them without swinging them into the personnel or the plane, and maneuver them into the brackets. Military sponsors expect that replacing current munitions-handling methods with ATTD-like systems will enable them to reduce staff and costs and increase efficiency by 200 to 500%.

The ATTD grasps a load with a control arm rather than pushing, pulling, or suspending it. The operator lifts and controls the load with a small joystick-type handle on the machine. The ATTD senses the motion and forces exerted by the operator's hand and duplicates the motion while amplifying the forces. Essentially, the machine follows every move of the operator's hand, but provides power that multiplies (by a preselected amplification ratio) the operator's strength. Many types of end-effector tools can be mounted on the end of the control arm—a gripper, a power tool holder, jaws, large parts, stretchers. The apparatus sits on an omnidirectional platform that also can follow the operator's movements, allowing easy transportation of the payload

François Pin, ORNL's principal researcher on the ATTD, notes that human amplification systems are usually envisioned (e.g., as in *Alien II*) as wrapping around the human operator. In an accident, however, the human strapped inside could be crushed. The ORNL machine is operated by a person standing beside it, delivering the benefits of amplification while avoiding the potential safety problems.

The striking difference between the ATTD and other materials-handling technologies is not the load it can lift, but rather the stability and control it provides: submillimeter-level precision with payloads of several tons. Cranes, for example, can handle huge payloads but cannot hold them stable, so accidents from hoisting with cranes are common.

The ATTD is a first demonstration system of controls technologies that balance the real forces on the payload and the virtual forces on the human operator. The operator needs to feel what is happening to the payload to sense inertia and know when the load has made contact; otherwise, the load could be dropped or crushed. However, the force the operator feels is greatly deamplified. The ATTD was tested at a 500 amplification level: The operator exerts 10 lb of force to move a 5000-lb payload. Machines could be designed to lift 50,000 lb with 10 lb of human force. The methodology lends itself to amplification ratios ranging from 1 to virtually infinity.

The ATTD relies on several ORNL-developed technologies, including new controls for hydraulic systems, human amplification, the omnidirectional holonomic platform, and high-precision control of large payloads. The existing system is hydraulic, but pneumatic or electrical systems also could be developed.

Although funding for the ATTD research has come from the armed forces, ORNL is discussing agreements with private companies that want their own systems. The technology is expected to have applications in fields such as manufacturing, construction, mining, emergency response, and other areas in which precise handling of large payloads is important. In an automobile plant, for example, one person using an ATTD-like machine could position engines in chassis. In a disaster such as the Oklahoma City bombing, clearing rubble using human amplification would be less dangerous to rescuers and survivors than clearing it with bulldozers.

Although its usefulness for boxing aliens has yet to be tested, enough is known about this new technology to lift the spirits of operators who move heavy payloads.

Development of the ATTD was supported by the U. S. Air Force, U. S. Navy, and U.S. Marine Corps.

François Pin uses ORNL's ATTD to hook a 500-lb unarmed bomb into the holding apparatus under an F-15 wing pylon. This prototype machine can lift and control a 5000-lb payload with 10 lb of human force, but the technology could be used to lift 50,000 lb with the same human force. *Photograph by Tom Cerniglio.*

Radioactive Tank Cleaning System Working at ORNL

The robotic system being used to clean out ORNL's gunite and associated tanks may help remediate DOE's other tank wastes.

Historical photograph of gunite tanks at ORNL (1943).

Imagine removing thousands of gallons of radioactive waste from an underground tank. Some of it is hard sludge, and some is contaminated scale stuck to the walls. You can't go inside the tank, and the only access is a few 2-ft-diameter openings in the top.

That's the situation the Department of Energy faces in trying to clean up cold war legacy wastes across its weapons complex. Hundreds of waste tanks containing millions of gallons of waste, some of it highly radioactive, must be emptied and scoured to eliminate the potential for leakage of contaminants into groundwater systems. The gunite and associated tanks (GAAT) project demonstrated the first successful cleanup of two underground tanks at ORNL in 1997–98 using the radioactive tank cleaning system (RTCS) developed and integrated at ORNL.

About 98% of the contamination from tanks W-3 and W-4 in the tank farm at ORNL was removed with the RTCS, says project manager Dirk Van Hoesen. The successful demonstration of the RTCS will reduce the original tank remediation schedule by 13 years and reduce the estimated cost by $120 million.

The GAAT project focuses on remediating eight tanks at ORNL, each 25 or 50 ft in diameter, built in the 1940s to store liquid radioactive wastes from the Graphite Reactor and radiochemical processing plant. The tanks were constructed with gunite (a concrete-like material) sprayed over a reinforcing grid.

The RTCS can characterize waste, dislodge it, pump it out, and then decontaminate the tank walls and floor once the waste is removed, all without the need for a person to enter the tank. It is the result of collaboration among several DOE laboratories, universities, and private companies. ORNL served as the design and development lead, coordinating efforts of all the participants.

The RTCS integrates several remotely operated tools. The waste dislodging and conveyance system uses an end-effector with rotating water-cutting jets to dislodge waste from the tank's interior. A jet pump removes the waste slurry from the tank through hoses. A modified light-duty utility arm (MLDUA) with 7 degrees of freedom, a 16-ft horizontal reach, and a 200-lb payload capacity can descend 50 ft vertically into a tank. The MLDUA can position the retrieval end-effector to clean the tank walls and floor. A remotely operated vehicle called Houdini has a 4 × 4-ft chassis that folds up to fit through a 2-ft-diameter tank entrance. Houdini has a bulldozer blade to break up debris and push sludge toward the retrieval end-effector, on-board cameras, and an articulated arm to pick up debris and manipulate other tools.

The Houdini (left) and MLDUA (center) are among the components of the RTCS that work together to effectively clean a tank's interior. *Image provided by the Gunite Tanks Remediation Project.*

The RTCS also includes tools to sample and characterize wastes and monitor radiation levels. Once the waste is dislodged and removed, the tank walls and floor are characterized to evaluate the depth to which contaminated materials have been absorbed. A scarifying end-effector is used to remove the layer of contaminated concrete. Remote cameras monitor tank cleanup, and the RTCS is controlled from a control trailer located near the tanks. The MLDUA can be controlled either manually or by preprogrammed sequences, and operators can switch back and forth seamlessly between the two modes.

ORNL's gunite tanks contain about 88,000 gallons of sludge. Tanks at other DOE sites have larger capacities and hold more sludge waste. The process at ORNL, part of the Oak Ridge tank remediation effort, serves as a pilot operation for the rest of the DOE complex; solutions can be worked out here on a smaller scale and tailored to fit specific needs at other sites. All sludge removed from the gunite tanks will be consolidated in one tank and then transferred by pipeline to the Melton Valley Storage Tanks (MVST).

Waste processing at the MVST is scheduled to begin in 2002. It takes 3 to 6 months to clean a tank and move the equipment to another tank. Finishing the GAAT project will take another three and a half years, Van Hoesen says. Just as the Graphite Reactor was a pilot for the nation's weapons program, the gunite tanks cleanup is a pilot for remedying its legacy of environmental contamination.

The project is funded by DOE's Office of Environmental Management.

Winning Big in the R&D 100 Awards Competition

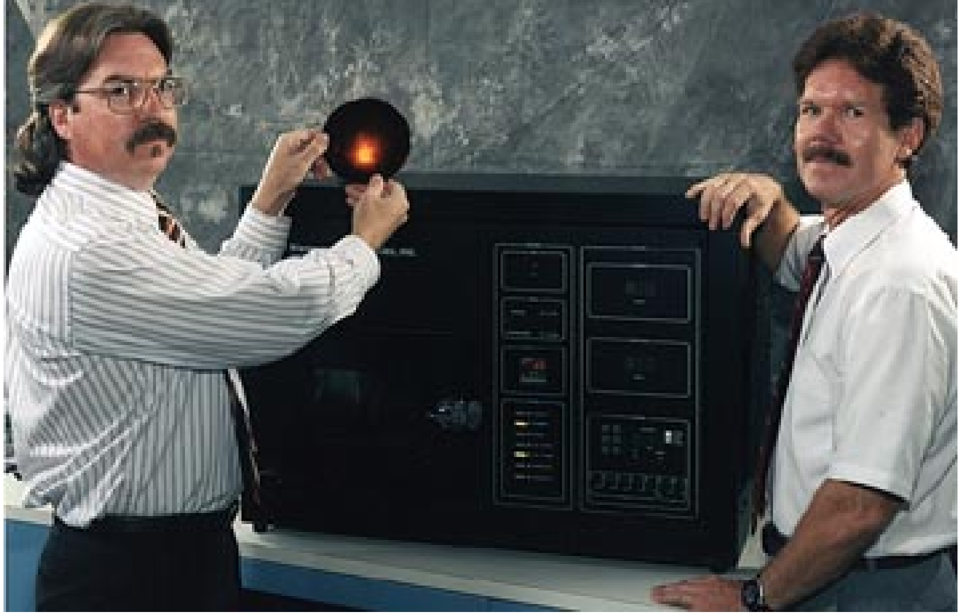
A system developed by (from left) ORNL's Russ Knapp, Saed Mirzadeh and Emory Collins improves upon conventional methods to produce technetium-99m, the principal radioisotope used in diagnostic nuclear medicine. The new method is environmentally cleaner, safer, and less expensive than conventional methods of producing the parent radioisotope, molybdenum-99, by fission of enriched uranium-235. *Photograph by Tom Cerniglio*.

In 1997 ORNL and Energy Systems had their best year yet in the R&D 100 Awards competition. Oak Ridge researchers won nine awards, pushing the Department of Energy's Oak Ridge total to 103 since the awards began in 1963. The awards are presented annually by R&D Magazine *in recognition of the year's most significant technological innovations. Winning inventions and inventers were*

- the High-Performance Storage System (HPSS) used for moving, storing, and retrieving large data files of high-performance computers and networked workstation clusters, developed by ORNL's **Randall Burris** and researchers at Lawrence Livermore, Los Alamos, and Sandia national laboratories and at IBM Global Government Industry;
- modular technetium 99-*m* concentrator for producing the diagnostic radioisotope without generating highly radioactive waste, developed by **Emory Collins, Saed Mirzadeh,** and **Russ Knapp**;
- production of succinic acid for making chemicals (e.g., food additives, paints, and plastics) by using a novel microorganism to ferment corn in a bioprocessing system, developed by **Brian Davison, Nhuan Nghiem,** and **Bruce Suttle** in a joint venture with Argonne National Laboratory, Pacific Northwest National Laboratory, National Renewable Energy Laboratory, and Applied CarboChemicals;
- cationic epoxy resins that are curable by electron beams (an alternative process for producing lightweight, fiber-reinforced plastics that uses less energy, works faster, emits less pollution, and

ORNL's Srinath Viswanathan (right) and Robert Purgert of Thompson Aluminum Casting Company of Cleveland developed metal compression forming, enabling the fabrication of pore-free cast aluminum alloy components that have properties comparable to those of forged parts at up to one-third the cost. *Photograph by Tom Cerniglio.*

ORNL's Amy Dindal and Mike Sigman developed methylated sol-gel sorbent, a product for detecting airborne pollutants such as carcinogens and industrial effluents. Because of its chemical and thermal stability, the new product is expected to do the job more efficiently and at lower cost than air sampling traps on the market. *Photograph by Tom Cerniglio.*



ORNL's Robert Lauf (left) and Don Bible developed the Vari-Wave, a flexible microwave heating system for laboratory research, analytical testing, and process development for industries producing or using advanced materials. Applications of Vari-Wave include processing advanced polymers and composites, as well as curing adhesives and encapsulants in electronic packaging assemblies. *Photograph by Curtis Boles.*

may be less costly than conventionally used thermal curing), developed by **Chris Janke, George Dorsey** (Y-12 Plant), Stephen Havens (ORISE), and Vincent Lopata (Atomic Energy of Canada);

- methylated sol-gel sorbent for detecting airborne carcinogens and other industrial pollutants, developed by **Michael Sigman, Amy Dindal,** and George Wachob of Supelco Incorporated;

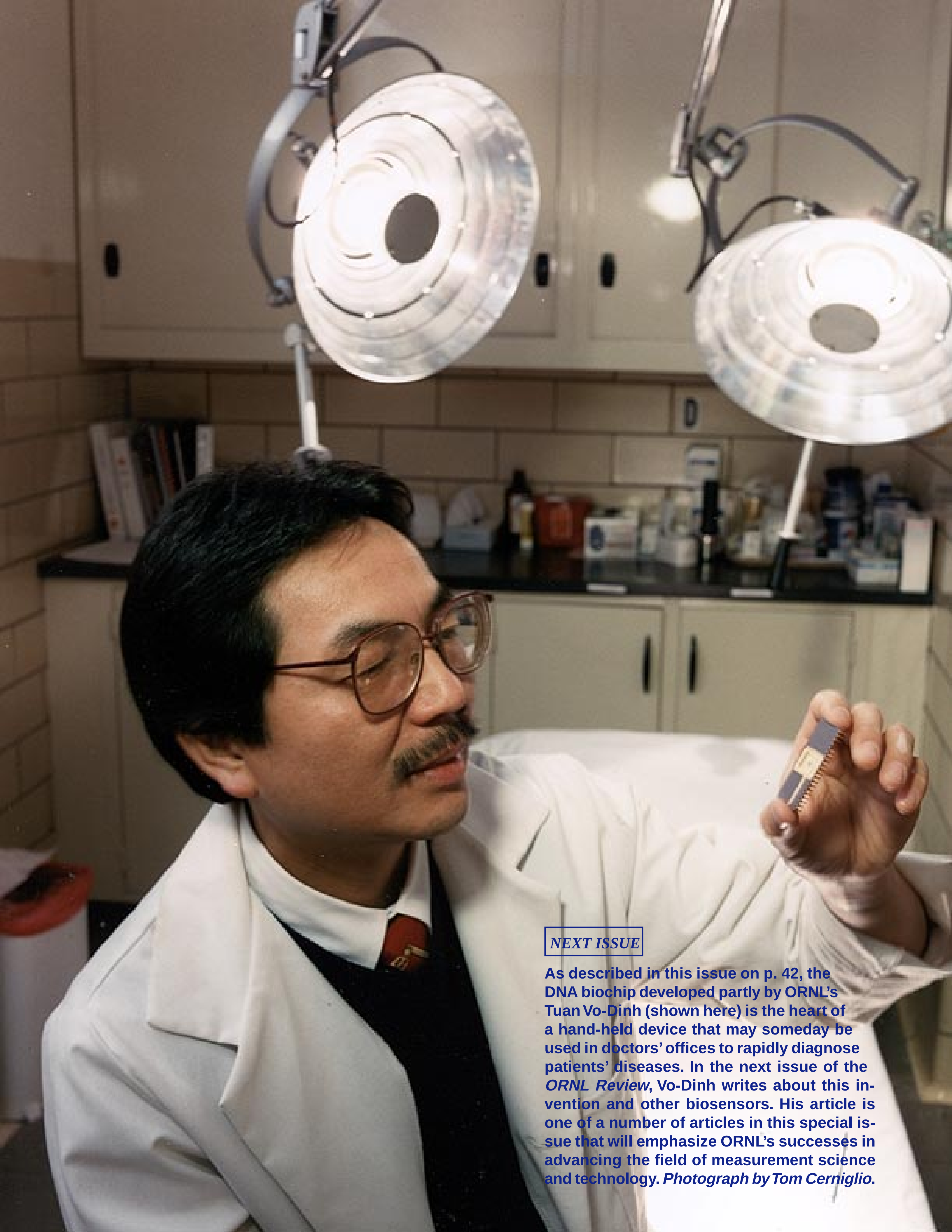
- metal compression forming used to make possible pore-free cast aluminum alloy components that have properties comparable to those of forged parts at up to one-third the cost, developed by **Srinath Viswanathan** and Robert Purgert (Thompson Aluminum Casting Company of Cleveland);

- Vari-Wave, a microwave heating instrument that dramatically reduces curing time (from two hours to three minutes) of adhesives and polymers used in the production of circuit boards and components, developed by **Bob Lauf, Don Bible** (both of ORNL) Zak Fathi, Mike Hampton, and Ralph Stevens, all of Lambda Technologies of Morrisville, N.C.;

- Enclosed Space Detection System that detects vibrations from the heartbeat of a person hiding in a vehicle, developed by **Leo Labaj, Michael Bath, Vivian Baylor, Michael Carroll, Mike Fuller, Tim Hickerson, Tom McCoig,** and **Richard Pack**, all of the Y-12 Plant, and by ORNL's **Bill Dress** and **Stephen Kercel**;

- carbon-free metal-ceramic composite crucible for melting high-purity metals, such as uranium and copper, using induction heating, developed by **Marvin Morrow** (Y-12 Plant), **James Kiggans, Jr. (**ORNL), **Cressie Holcombe** (retired from Y-12 Plant), and Don Rexford of Blausch Precision Ceramics of Albany, New York.

ORNL's Randall Burris teamed with researchers at Lawrence Livermore, Los Alamos, and Sandia national laboratories and at IBM Global Government Industry to develop the High-Performance Storage System (HPSS). HPSS is designed to manage enormous amounts of data produced and used in modern high-performance computing, data collection and analysis, imaging, and enterprise environments. *Photograph by Tom Cerniglio.*



NEXT ISSUE

As described in this issue on p. 42, the DNA biochip developed partly by ORNL's Tuan Vo-Dinh (shown here) is the heart of a hand-held device that may someday be used in doctors' offices to rapidly diagnose patients' diseases. In the next issue of the *ORNL Review*, Vo-Dinh writes about this invention and other biosensors. His article is one of a number of articles in this special issue that will emphasize ORNL's successes in advancing the field of measurement science and technology. *Photograph by Tom Cerniglio*.

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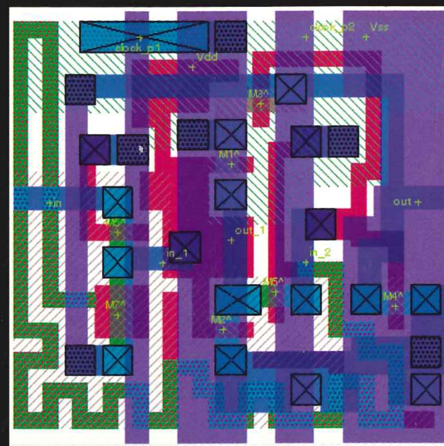

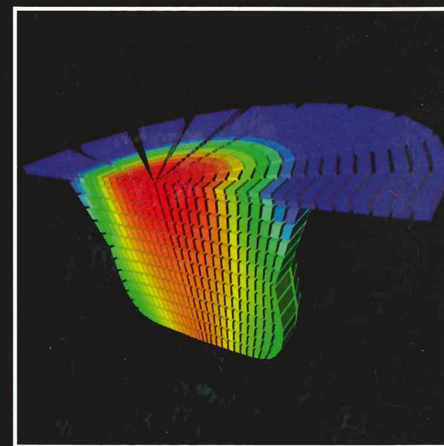

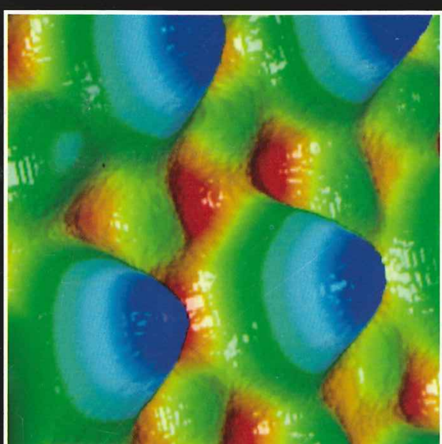

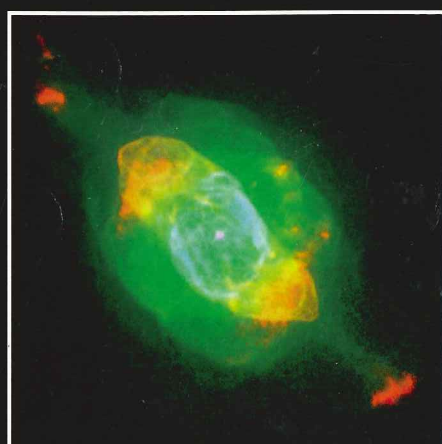

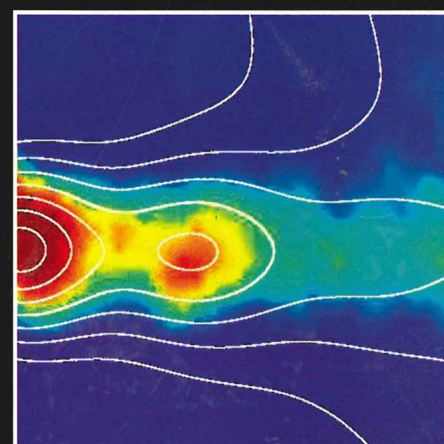

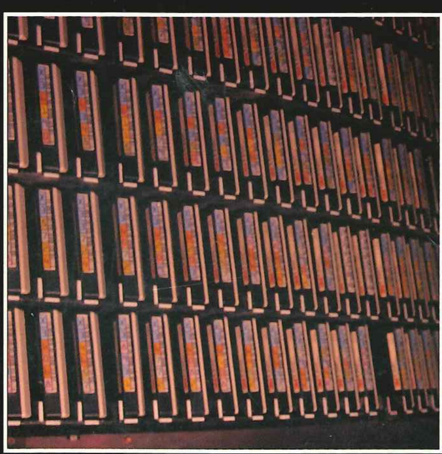

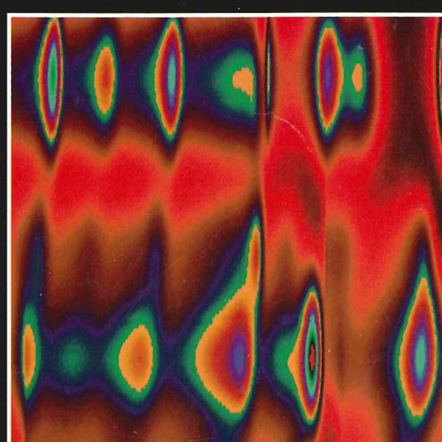

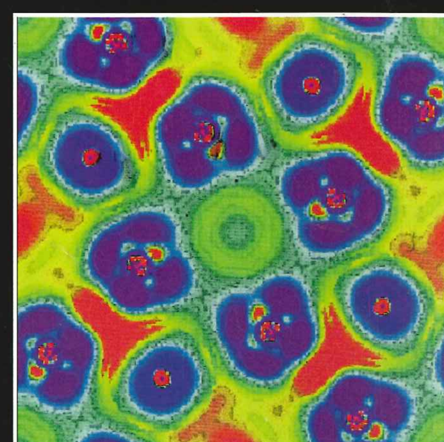

See inside for the stories behind these images.

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