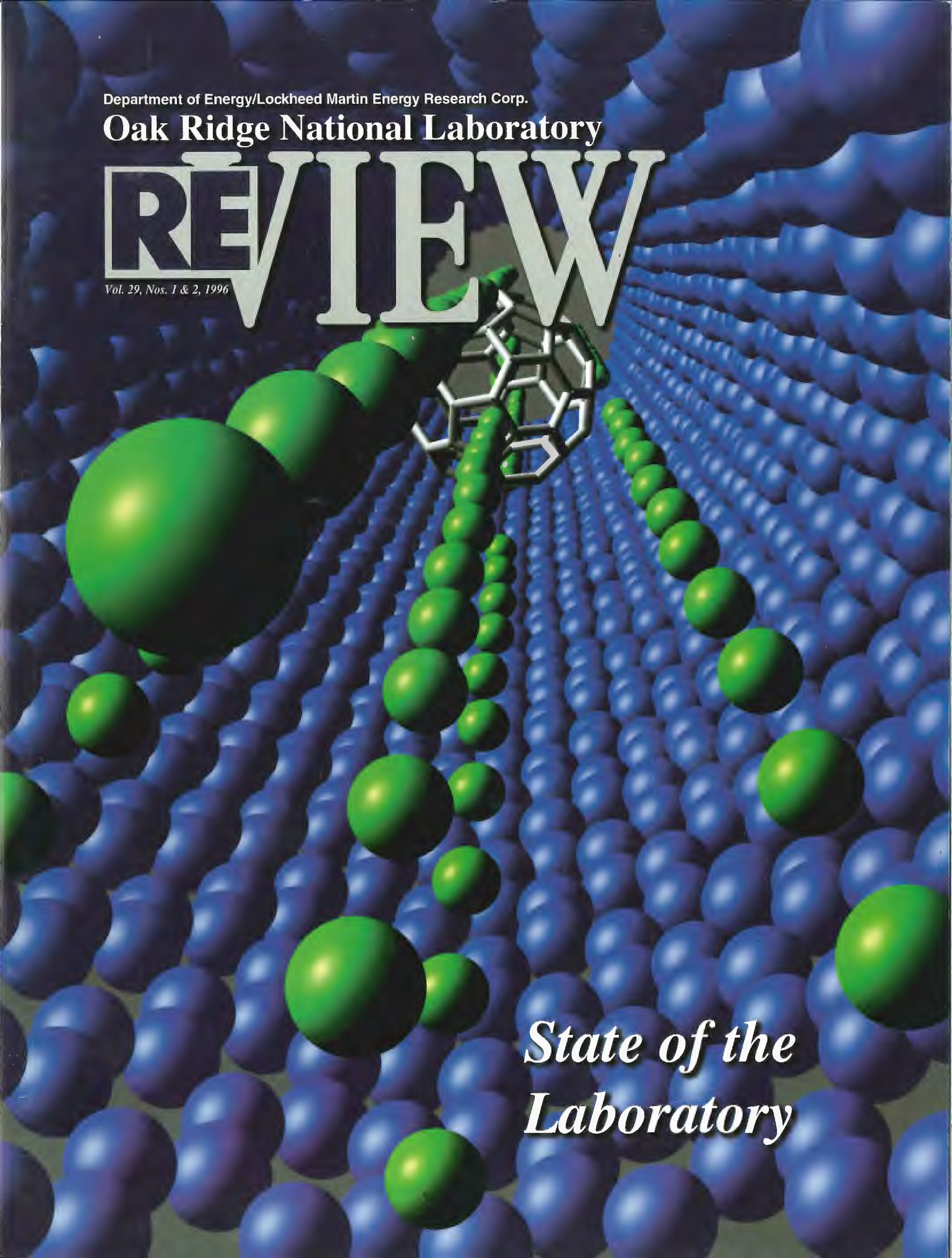
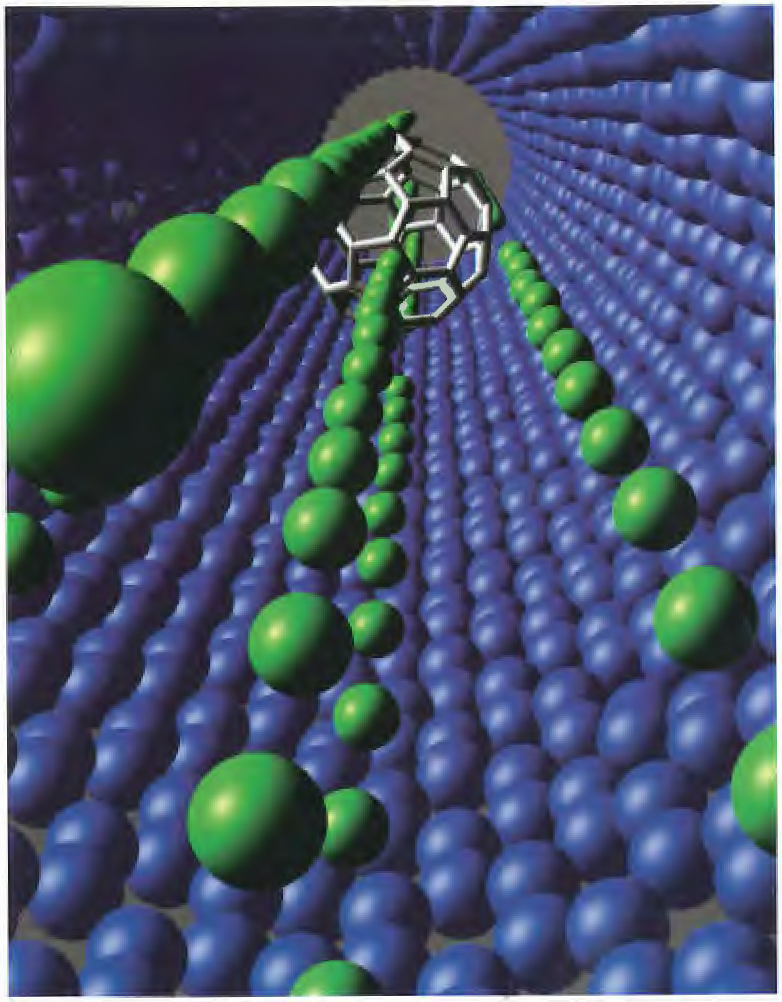
Department of Energy/Lockheed Martin Energy Research Corp.

Oak Ridge National Laboratory REVIEW

Vol. 29, Nos. 1 & 2, 1996



State of the Laboratory



COVER CAPTION

Visualization of helium flow pushing a "buckyball piston" in an all-carbon nanotube (see p. 79). It is one of ORNL's many research highlights in 1995 that are presented in this State of the Laboratory issue. The molecular simulation was performed by Donald W. Noid, Bobby G. Sumpter, and Robert E. Tuzun, all of ORNL's Chemical and Analytical Sciences Division. The visualization was produced by Ross Toedte of the Center for Computational Sciences Visualization Laboratory. The cover was designed by Vicki Beets, graphic artist in the Computing, Information, and Networking Division.

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

Editor
Carolyn Krause

Assistant Editor
Deborah Barnes

Consulting Editor
Bill Appleton

Writers
Carolyn Krause, Susan Fisher,
John Getsi, Walter Koncinski

Designer
Linda Dickert

Electronic Publishing
Vickie Conner, Gloria Glandon, Sandra Lyttle

For more information, contact
Joe Culver
4500-North, M.S. 6266, Oak Ridge, TN 37831-2008;
telephone: (423) 576-0235; FAX, (423) 574-0595;
or electronic mail, culverjw@ornl.gov.

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

The address of our editorial office is Building 4500-South, M.S. 6144, Oak Ridge, TN 37831-2008; telephone: (423) 574-7183 or (423) 574-6974; FAX, (423) 574-1001; electronic mail, krausech@ornl.gov.

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
Computing, Information, and Networking Division.

REVIEW
Vol. 29 Nos. 1–2, 1996

Contents

p. 13

2 State of the Laboratory Address

10 Life Sciences Initiative
Gene Function Research

12 Neutron Science and Technology Initiatives
Oak Ridge Spallation Neutron Source
High Flux Isotope Reactor Upgrades

20 Biological Sciences

29 Environmental Sciences and Technology

35 Energy Production and Energy End-use Technologies

44 Instrumentation, Manufacturing, and Control Technologies

53 Advanced Materials Processing, Synthesis, and Characterization

63 Physical Sciences

70 Computational Science and Advanced Computing

80 Robotics

81 Educational Activities

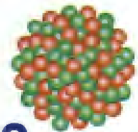
82 Development and Operation of National Research Facilities

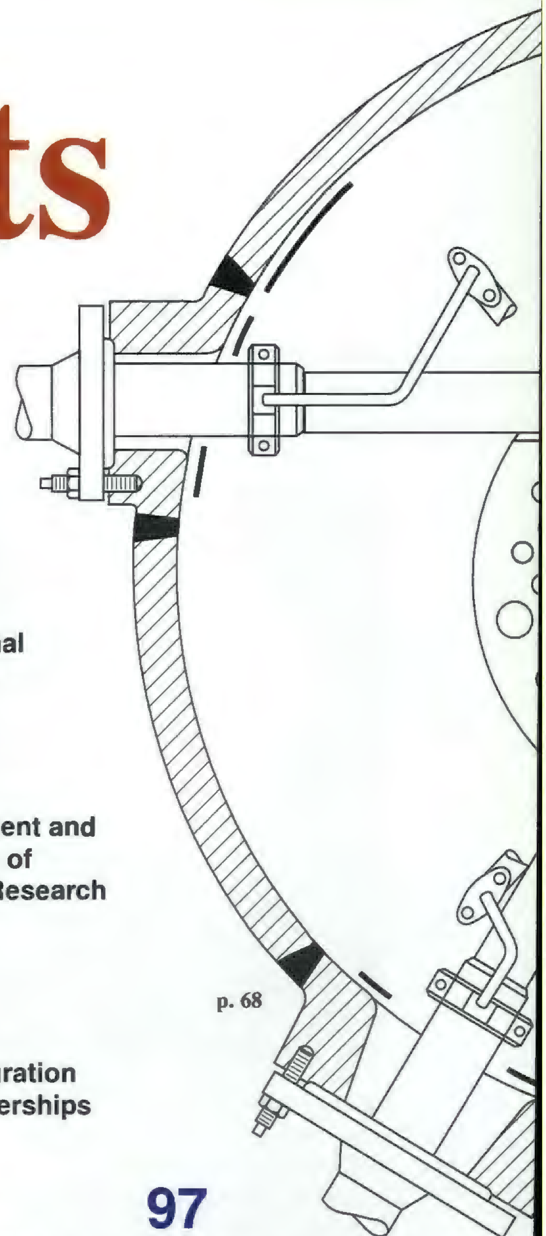
89 R&D Integration and Partnerships

91 Operations and Administration

97 Technology Transfer: CRADAs, Licenses, and Patents

105 Awards



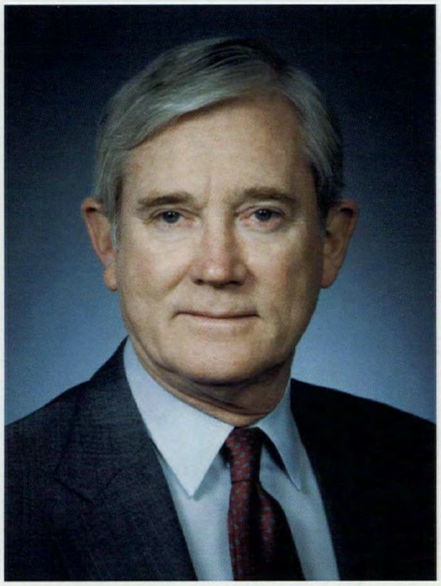


p. 68

p. 20

For the first time an ORNL experiment blasted off aboard the U.S. Space Shuttle Columbia, . . . The idea . . . was to grow near-perfect crystals of chromosome building blocks called nucleosomes by capitalizing on the absence of gravity in outer space. It is believed such crystals will grow more slowly, making them defect-free, solid instead of hollow, more uniformly shaped, and larger than nucleosome crystals grown on earth.

State of the Laboratory—1995



Alvin Trivelpiece tells ORNL employees what the Laboratory needs to do to ensure its survival. *Photograph by Curtis Boles.*

Editor's note—ORNL Director Alvin W. Trivelpiece delivered his annual State of the Laboratory address to employees and visitors on April 26, 1996, in Eugene P. Wigner Auditorium, Oak Ridge National Laboratory.

I am pleased to note that we have in the audience two former directors of Oak Ridge National Laboratory—Herman Postma and Alvin Weinberg; the president of Lockheed Martin Energy Systems, Gordon Fee; and the manager of the Oak Ridge Operations Office, Jim Hall.

In previous years, I have talked about some of the comings and goings of a few people in various positions around the Laboratory. I have also talked about prizes and awards that have been received by various members of the scientific and technical staff, and I have tried to explain some of the interesting research and development (R&D) work that has been done around the Laboratory during the past year.

This year, I will instead outline important events that have shaped our institution during the past year and I will discuss what I believe they mean in terms of the health and well-being of Oak Ridge National Laboratory.

I am also going to outline some of the actions that I believe we must take to survive and prosper as an institution. There are many forces at work over which we have little or no control. Such forces may have profound effects on our future.

I have one piece of good news. The President has signed the '96 budget into law. I hope that this action spurs the Congress to pass a '97 budget before October 1.

I gave last year's State of the Laboratory address on March 3. Nothing in that talk predicts anything that actually happened to us since then. So in giving this State of the Lab talk, I want to make it clear that my ability to predict the future is bad.

I don't need to tell most of you that a lot has happened at ORNL this past year. Even so, I suspect that many of you haven't thought about what it all means to us as an institution. Some of these events have already changed us a great deal. Some of the forces that led to these events will continue to be imposed on us. How we respond to these forces will determine how well Oak Ridge National Laboratory continues to survive and prosper as a leading research and development (R&D) institution.

I am going to divide my remarks into three parts. First, the way we were; second, the way we are; and third, the way we need to be.

How we respond to these forces will determine how well ORNL continues to survive and prosper as a leading research and development institution.

Lockheed Martin Corporation's Dan Tellep (left), chief executive officer, and Norm Augustine, president, visit with ORNL employees in March 1995. *Photograph by Jim Mottern.*

The Way We Were

In 1993 we celebrated the 50th anniversary of the events that began what is now known as Oak Ridge National Laboratory. This celebration provided a great occasion for us to reflect on the way we were. Several books have described the birth of the Laboratory during World War II and the activities here as part of the war effort. Then all of a sudden the war was over, and the question was, "What next?"

Major General Leslie R. Groves' Advisory Committee on Research and Development met on March 8 and 9, 1946, in the New War Department Building, Washington, D.C., to consider the future. Because the new commission could not be formed in time for the fiscal year 1946-1947, it was assumed that the Manhattan District would continue in existence temporarily and that it would request funds for certain R&D programs. One of the subjects of this advisory committee meeting was "national laboratories."

No precise definition of what a national laboratory should be was made by this advisory committee, or by anybody else since then for that matter. The conditions laid out in the minutes of the Groves Advisory Committee meeting indicate that the R&D work undertaken in national laboratories should be primarily fundamental research of an unclassified nature requiring the use of piles and equipment of too great a cost for a university or private laboratory to underwrite. They recommended that the work at the Clinton Laboratories be continued.

In 1947, the scientists and engineers here at the Clinton Laboratories were pleased to learn that the University of Chicago would most likely succeed Monsanto as the contractor. However, after Christmas of 1947, they were then disappointed to learn that, instead of the University of Chicago, the contractor was going to be a subsidiary of Union Carbide and that reactor development was going to be centralized at the Argonne National Laboratory instead of at Oak Ridge. Even so, there were forces at work that would change this situation very quickly. In January 1948, the Atomic Energy Commission (AEC) changed the name of our institution from Clinton Laboratories to Oak Ridge National Laboratory.

In March 1949, Alvin Weinberg wrote a then classified report, *Research Program at ORNL*. The leading line of that report says, "The activities of Oak Ridge National Laboratory fall into six large categories: chemical technology, reactor technology, basic research, isotope production, radiation protection, and education." We are still doing some of these things. However, it is a later section of the report that reveals for the first time some clue about how frustrating it can be to deal with the problems of running a national laboratory. Weinberg wrote, "ORNL continues to produce important work for the AEC, in spite of a combination of circumstances which included two changes of contractor, a drastic change in directive (sic), and 14 months during which there was no research director." From this I conclude that it must have been nice to be able to keep material classified until after you could retire.

Over the years since then, the fortunes of ORNL changed with the times, and the thrust of its programs changed as a result. The 1973 oil embargo gave impetus to work in areas of energy research other than nuclear energy. National concerns over the environment led to opportunities for new areas of research at ORNL. The Calvert Cliffs decision spawned considerable work in preparing environmental impact statements that

Former ORNL Director Alvin Weinberg (left), who celebrated his 80th birthday in 1995, meets with Clifford Shull, who spoke at ORNL shortly after winning the Nobel Prize in physics for his neutron scattering research more than 40 years ago at the Laboratory's Graphite Reactor. *Photograph by Curtis Boles.*

comply with the National Environmental Policy Act. Ecological sciences here got a boost.

In 1975, the AEC was replaced by the Energy Research and Development Administration, which in turn was replaced by the Department of Energy in 1977. With the establishment of the Department of Energy, management attention was now directed to how national laboratories were operated, as well as to what they did. This scrutiny resulted in a management structure that was not as lean as the AEC.

There were also changes in DOE-supported scientific and technical programs and in the manner in which they were funded. Programs in various areas of conservation and renewables were expanding. The controlled thermonuclear fusion program grew for a while. Fossil energy research was increased greatly. The Three Mile Island nuclear plant accident occurred. Support for development of nuclear power expanded and then began to diminish.

Even though these changes in directions in our technical programs were substantial, they were normal in the sense that an R&D institution should expect to be doing new and different things. But in looking back, probably the biggest change in the operation of Oak Ridge National Laboratory during this 40-year period occurred not as a result of routine changes in technical direction. Rather, the biggest change was the transition from a fixed-fee contract to an award-fee contract. This change occurred when Martin Marietta won the competition for operation of the Oak Ridge facilities, effective April 1, 1984. At the time this did not seem like a big change. The award fee levels were not substantially different from the previous fixed fees, and the primary criterion by which the Lab's performance was judged was scientific excellence.

DOE Secretary Hazel O'Leary visited Oak Ridge during the Oak Ridge Summit on June 1 and 2, 1995. During the Summit, the Basic Research Subcommittee of the House Committee on Science heard testimony on the challenges facing scientists in Oak Ridge, Tennessee, and the nation. *Photograph by Lynn Freeny.*

The biggest change was the transition from a fixed fee contract to an award fee contract.

However, in the late 1980s, concerns over management issues grew. As a result, award fee performance measures were changed to give greater emphasis to management concerns instead of scientific performance. Also, certain functions were centralized and managed by individuals no longer accountable to Laboratory management. At one point, it was estimated that more than 90% of the Lab's award fee performance was based on its adherence to management directives rather than on the excellence of its scientific and engineering work. After some negotiations, this balance was changed so that it was based only 60% on management performance. In any event, I did not believe that such a focus on management performance was a proper way to run a national laboratory, any national laboratory.

As a result of this situation, morale suffered, scientific productivity dropped, costs soared, and our program sponsors were becoming dissatisfied with us to the point of threatening to shut down funding for several key programs. All of these happy events occurred within the first couple of years after I was named Laboratory Director. There were probably a few things that my predecessor, Herman Postma, meant to tell me about the Lab before I came here, but they probably just slipped his mind.

What was obvious in early 1992 was that this process had caused our overhead costs to get out of control; thus, the only way we were going to stay in business was to bring them under control. The first difficult step in this process was to establish Project 45, which sought to bring our projected overhead rate of 54% down to 45%. It was a critical and painful first step. The process continues and has a way to go.

Later in that same year on November 12, the Lab's executive committee was at an offsite meeting in Townsend, Tennessee. We took time out from our discussion to listen to President-elect Clinton's first press conference after his election. He introduced some of his early appointments and then made the following remarks at the Old State House in Little Rock, Arkansas.

"I have read at least in my history books that some cabinet appointments are considered major and others are considered minor. I don't know how you would consider the Departments of Commerce and Energy in that regard, but from the kind of economic policy I have laid out, and the things that I think we have to do to change this country economically, those are very major appointments. And how they pursue the missions of those departments will affect the success or failure of this administration's economic efforts, as well as what is done by the other major economic players."

Fantastic! What could go wrong after the president-elect said that the Department of Energy was critical to his administration's success?

Well, neither we nor President Clinton had yet to observe the character of the 103rd Congress that was to be sworn in in January 1993. Their logic seemed simple enough. The Cold War is over. We don't need to make any more nuclear weapons. The DOE labs make nuclear weapons, so they should be shut down. Which ones? Why not use the base closing commission approach? Several bills were introduced that proposed this course of action. Others called for the examination of the roles and missions of the national laboratories. None of these bills was introduced with the notion that the roles and missions should be expanded. Other proposed legislation focused on the concern over the way that our Laboratory Directed Research and Development activities were carried out. There was also concern over whether our work for other federal agencies shouldn't be done by the private sector. There was concern that the expected technology transfer from the labs wasn't occurring fast enough and that, if it was, it was benefiting other countries.

To her credit, Secretary of Energy Hazel O'Leary recognized these and other forces that were threatening the Department and its laboratories. In response to these threats, she asked Bob Galvin, chairman of the board of directors at Motorola, to lead a Task Force on Alternative Futures for the DOE Laboratories. The Task Force began its work in February 1994 and presented its findings and recommendations in February 1995. The Galvin Task Force report gave a good analysis of the situation regarding the operation of the labs and of the Department. It was done in a fair and

Ribbon cutting for the new Solid State Division building. From left are physicist Doug Lowndes, ORNL Associate Director Bill Appleton, ORNL Director Alvin Trivelpiece, Ron Hultgren (DOE site manager at ORNL), Solid State Division Director Jim Roberto, and crystallographer Lynn Boatner. *Photograph by Curtis Boles.*

objective manner and there was no basis for objection to its conclusions and findings.

After receiving the Galvin Task Force report, Secretary O'Leary set out to implement most of its recommendations. In spite of her actions, there were still strong forces that wanted to abolish the Department of Energy. In response to these continuing threats to the Department, Secretary O'Leary announced in late 1994 that she was going to have a strategic realignment program for the Department. This realignment would involve a 25% reduction in federal employees over five years. The Department is now down to 13,000 employees from over 19,000 just a few years ago. The realignment would also require a reduction in the cost of operations at the Department's national laboratories by about $1.4 billion over the same five-year period. ORNL's fair share amounts to reducing our costs of operation by about $18 million each year for a period of five years. This is not an easy target for us and we could not meet it without the firm commitment by Secretary O'Leary to push the "necessary and sufficient" approach to regulatory reform.

I believe that if Secretary O'Leary had not proposed her strategic realignment, the Department of Energy might well have been abolished by now. But we should keep in mind, the forces that led her to carry out this strategic realignment have not gone away. There are still several pending bills in the Congress that propose to abolish the Department of Energy.

The Way We Are

All of this was very dramatic. Working with the Galvin Task Force was a very time-consuming but worthwhile effort. A lot of you had a chance to participate. However, there are several other entities that also have great influence on what we do besides the Department of Energy. These other entities have also been undergoing profound changes as a result of the cessation of the Cold War. In particular, the Department of Defense. There have been major reductions in the armed forces and a corresponding reduction in the procurements of items that companies like Martin Marietta supplied. Norm Augustine, then chairman and chief executive officer of Martin Marietta, decided that merging with another company was a superior strategy for the future instead of going out of business. This approach led to the acquisition of GE Aerospace. Martin Marietta was now a $10 billion company.

Then, Mr. Tellup, chairman of Lockheed, also a $10 billion company,

Tennessee Representative Zach Wamp and Martha Krebs, director of DOE's Office of Energy Research, played prominent roles during the Oak Ridge Summit. ***Photograph by Lynn Freeny.***

and Mr. Augustine agreed that a $20 billion company was better than two $10 billion companies. The complementary nature of the activities of the two organizations made this a very strategic merger. This merger did leave a few areas where neither company had strengths that would be desirable for a full service defense and aerospace contractor. This need will be met by the recently approved integration with Loral Corporation. We will now be part of a $35 billion corporation when you take into account the $5 billion in equivalent sales represented by the various DOE facilities such as ORNL.

Most of these changes occurred after the last State of the Laboratory Address on March 3, 1995. March 15 was the day that Lockheed Martin Corporation was born. The way by which a $20 billion corporation is managed is substantially different from the way a $5 billion corporation is managed. Lockheed Martin established four sectors, each with its own president to manage most elements of the company. The elements of the company that were not part of one of the four sectors included Sandia National Laboratories, Idaho National Engineering Laboratory, Lockheed Martin Energy Systems, and others that had not been assigned to a sector. It was decided that there should be a fifth sector and that Al Narath would be its president. On August 15, 1995, Al Narath announced that Oak Ridge National Laboratory would be separated from Lockheed Martin Energy Systems and that a new subsidiary company would be established to manage ORNL on a fixed-fee basis. On Friday, October 13, 1995, at 3:15 p.m., the Lockheed Martin Energy Research Corporation was chartered in the state of Delaware. On December 6, a new contract with the Department of Energy was signed. We started operation of the Lab under the new company on January 1, 1996. Between August 15 and December 31, a lot of hard work was done by a lot of people to make the new arrangement possible.

Prior to the proposal to establish a new company to manage ORNL, the Office of Energy Research in the Department of Energy was planning to have the Laboratory put out for bid, with only not-for-profit organizations such as universities being allowed to compete. I am glad that an alternative was found that allowed the contract with Lockheed Martin to be extended so that the Laboratory was not competed. I believe that our present arrangement is much better than being put out for bid. But make no mistake, we are on probation with the Department. Unless we perform up to the expectations of the Office of Energy Research and the other elements of the Department that have a say in our future, we might yet end up being put out for bid. I remain concerned that if we are to be

Howard Baker (center), former U.S. Senator from Tennessee, visits the Holifield Radioactive Ion Beam Facility at ORNL. His hosts are Jerry Garrett, right, and Michael Smith. ***Photograph by Curtis Boles.***

Neal Lane (right), director of the National Science Foundation, delivered a lecture in 1995 at ORNL. Here he autographs a poster announcing his visit in the presence of Nancy Gray, ORNL protocol officer, and Ed Oliver, an ORNL associate director. ***Photograph by Curtis Boles.***

competed, then we might just be shut down instead.

But even though we are not out of danger yet, we must also keep in mind that this transition to Lockheed Martin Energy Research had the firm and unwavering support of Dr. Martha Krebs, director of the Office of Energy Research at the Department of Energy. Without her support none of this would have happened. Many of you had the chance to hear her, when she visited us on January 11, 1996. She told us how pleased she was that the transition had occurred, and she congratulated us on what we had accomplished. You also heard Al Narath, president of the Lockheed Martin Energy and Environment Sector, express his commitment to help us succeed. Jim Hall, manager of the Oak Ridge Operations Office, and I signed an agreement that pledged us to work together in ways that improve the management and operations of both institutions.

Given this support and good will, I am optimistic about the future of Oak Ridge National Laboratory. We still have a lot of hard work yet to do to complete certain elements of the transition and find our own ways to do things in some areas of management. We have to get better in several areas in order to be able to compete in the current environment. That leads me into some comments on what we need to do to succeed.

The Way We Need To Be

January 3, 1996, was the first time I had the opportunity to tell you about events surrounding the formation of and transition to the new company. At that meeting, I told you about my expectations based on what I knew at the time. Since then, we have heard from Martha Krebs, Al Narath, and Jim Hall about their expectations. We have started a process of reengineering to determine how we can reduce costs and remain competitive in our principal lines of business. We have debated among ourselves about what we should do. We have sought advice from a lot of our friends about what we might do to improve ourselves. This is not an easy process. What follows is a list of what I believe to be the ten most important things we need to do. I have no illusion that this list will be accepted without challenge or question. It is the nature of this institution to challenge everything.

1. We need to build on the historic strengths and accomplishments of Oak Ridge National Laboratory to ensure that it will continue to be an outstanding research and development institution.

2. We need to commit ourselves to delivering scientific and technological value to the Department of Energy and to the nation and, in so doing, be second to none.

3. We need to be an institution that is so well regarded for its dedication to

It is within our ability to improve our chances for a better future with skill, a little cunning, and a lot of hard work.

Linda Horton explains a materials research advance at ORNL to Joseph Stauch, counsel general of South Africa, who visited the Laboratory in May 1995. *Photograph by Curtis Boles.*

excellence, for its unquestioned commitment to ethics, and for its record of integrity in all of its transactions that others regard us as the standard by which to be judged.

4. We need to be the most efficient and cost-effective Department of Energy national laboratory.

5. We need to recruit and retain a diverse and talented work force, because it is the people that make a great institution, not the bricks and mortar.

6. We need to strengthen partnerships with universities, industry, other Department of Energy laboratories, other federal agencies, and state and regional organizations in such a way as to leverage resources and create new opportunities.

7. We need to have a values program that is taken seriously.

8. We need to aggressively seek funding for the kinds of scientific and engineering facilities that will make us unique in certain areas of research and development critical to the Lab's future.

9. We need to communicate to taxpayers that what we do is of value to them and the nation and that we appreciate their support.

10. We need to deliver on our commitments to Lockheed Martin and to conduct our business in such a way that they are proud to have us as a member of the corporation.

This list of 10 is not unique. I hope that it leads to debate and discussion on what needs to be done. I expect it to be improved, modified, and acted on in many areas by this time next year.

I believe that, although the state of the Lab may be a bit uncertain and we are in for some difficult times, it is nevertheless within our ability to improve our chances for a better future with skill, a little cunning, and a lot of hard work.

I would like to close by paraphrasing a remark that Sir Isaac Newton made in a letter to Robert Hooke in 1675. In this letter he is speaking to both Hooke and René Descartes and is explaining to them why he had been able to do the remarkable things that he did when others like them had not. Newton wrote, "If I have seen further it is by standing on the shoulders of giants."

If Oak Ridge National Laboratory has seen further, it is because it stands firmly on the shoulders of the talented people who make up this outstanding institution. **ornl**

Gene Function Research

You have a unique identity, home address, and body structure. So does every human gene. The current emphasis of the Human Genome Program, co-sponsored by the Department of Energy, has been to determine the identity, location, and sequence of the chemical building blocks of each of the estimated 80,000 genes in the human genome. Now that more is known about where genes are and what they look like, ORNL is positioning itself for the next logical step of the program—finding out what genes do. When information on the entire human genome becomes accessible, experiments on gene function can be approached on a whole genome basis, not just one gene at a time—hence the term "functional genomics."

Lisa Stubbs and colleagues gain valuable information from ORNL's mouse collection. *Photograph by Tom Cerniglio.*

In a sense, the Human Genome Program is developing a "telephone book" that lists the name, address, and phone number of each of the human genes. For the science of functional genomics, biologists will use the "phone number" for each listed gene to "call up" groups of genes to ask questions about what they do—through gene function experiments. ORNL has the experts and model organisms to use this limited information to link the location and structure of genes to the actual function they control (e.g., breathing).

Functional genomics has become a goal of ORNL's efforts because our researchers both have proven proficiencies in analyzing the functions of genes and have developed technologies that can be used to facilitate these experiments. In the past, we first learned about mouse genes by exposing mice to radiation and observing body changes (e.g., altered fur color) that could be related to altered genes. Similar mutations were produced in mice at ORNL, using chemical agents. Today, we produce mouse mutants through both chemical mutagenesis and a form of genetic engineering called targeted mutagenesis. In this technique, we "make" new mice by inserting an engineered gene into a mouse in the embryonic stage, ultimately causing a disruption of the corresponding gene in the host animal. If the disruption causes an abnormality, impaired function, or a disease in the mouse, then it is possible to determine which gene is partly responsible for the defective trait or function (e.g., a poorly working kidney). At ORNL "mouse models" for polycystic kidney disease, Type II diabetes, sickle cell anemia, cleft palate, genetic-based obesity, immunological defects, neurological disorders, and many other conditions have been developed. The information they provide about altered gene function could lead to a cure for at least one human genetic disease.

A new ORNL initiative in functional genomics, which will be supported by internal funding for the next four years, will enhance the Laboratory's capabilities in support of the DOE mission. With a focus on mouse mutagenesis, the functional genomics initiative will build on our expertise in mouse mutagenesis and our extensive mouse mutant resource being maintained in the Biology Division—our unique colony of more than 120,000 mice. In a broader sense, it will combine ORNL's expertise in

ORNL is positioning itself for the next logical step of the program—finding out what genes do.

mammalian genetics with our competencies in structural biology, computational sciences, robotics, automation, and instrumentation development. Integration of the expertise of molecular biologists with computer scientists and mathematicians is particularly important because analysis of the sequences of whole genomes has been hastened by creation of new algorithms and other mathematical feats. Our biologists' collaborations with computer scientists, analytical chemists, and engineers is providing highly productive experimental capabilities and technological breakthroughs for genetics research.

ORNL also has strong capabilities in analyzing structure and function of proteins, or gene products. Mutations of genes in living organisms give rise to mutated proteins that must be isolated and characterized to understand their consequences in the body. Mutated proteins encoded by relevant genes can also be generated in the laboratory by both chemical and genetic means. Protein engineering through recombinant DNA technology enables rational redesign of protein structure. This powerful approach will enhance our ability to understand protein function and tailor the properties of proteins in animals and plants for use in medicine, industry, agriculture, and biotechnology.

Our research in functional genomics will help us continue our tradition of successes in the biological sciences, thereby serving the needs of DOE and our society, and it will facilitate expanded outreach and partnerships under industry and academia. These multidisciplinary achievements, which bridge basic and applied research, have been honored by two Enrico Fermi Awards from DOE and more than a dozen memberships in the National Academy of Sciences.

Thanks to our mice and other research tools, we have discovered that health effects of radiation exposure are related to the intensity of the doses and that radiation is especially harmful to embryos in the early stages of development, prompting rules limiting the use of X rays on pregnant women. We found that the presence of a Y chromosome specifies male gender and that only one of two X chromosomes in a cell is active. We performed the world's first experimental bone-marrow transplants in mice. We performed the world's first successful freezing, thawing, and implantation of mouse embryos, which were brought to term in surrogate mother mice, establishing the basis for modern animal breeding and human fertility treatment.

Apart from mouse genetics, we have enjoyed other stunning successes: the first analytical separation of the building blocks of DNA and RNA, codiscovery of the nucleosome (the basic structural component of chromosomes) and low-level resolution of its structure by X-ray crystallography, codiscovery of messenger RNA (which conveys genetic information to the protein-synthesizing apparatus in all cells), discovery of biochemical pathways for repairing damaged DNA (thereby preventing mutations and cancers), rational design of enzyme inhibitors (a cornerstone of drug discovery), and development of the zonal centrifuge (for production-scale preparation of vaccines).

As an extension of these studies, we are attempting to unravel the role of RNA in the regulation of cell growth and differentiation. We are exploring the use of antibodies to deliver chemotherapeutic agents to certain organs or cell types. We are also using sophisticated techniques of genetic engineering to systematically redesign proteins found in nature in the hope of improving biomass yields (for food and energy) and developing effective drugs for treating cancer.

Fortunately, DOE's Office of Health and Environmental Research is an advocate and sponsor of our research. This support should help us not only play an important role in the second stage of the Human Genome Program but also contribute to the multifaceted missions of DOE in the life sciences. ornl

Brad Yoder examines mouse embryos that turn blue, indicating the expression of the disrupted gene that causes polycystic kidney disease. ***Photograph by Tom Cerniglio.***

Neutron Sources

Because isolated neutrons do not occur in nature, they must be extracted from atomic nuclei for use in scientific research. One source of neutrons is the nuclear fission process in a nuclear reactor. A second method of obtaining neutrons is spallation—bombarding nuclei of heavy atoms with energetic particles (usually protons) from a high-energy accelerator. When protons collide with target nuclei, 20 to 30 neutrons are knocked out, or "spalled," from each nucleus—thus the term "spallation."

Neutron sources have become invaluable tools for fundamental science, perfection of new industrial products, medical and biomedical applications, commercial power development, and defense purposes.

ORNL has a long history in using neutron sources for research. Because of the early neutron scattering research performed at ORNL's Graphite Reactor, a former ORNL researcher (Cliff Shull) received a 1994 Nobel Prize in physics. Today neutron scattering research is conducted at ORNL's High Flux Isotope Reactor (HFIR), which has the world's highest thermal neutron flux; about 290 users annually do neutron research at the HFIR, which is 30 years old.

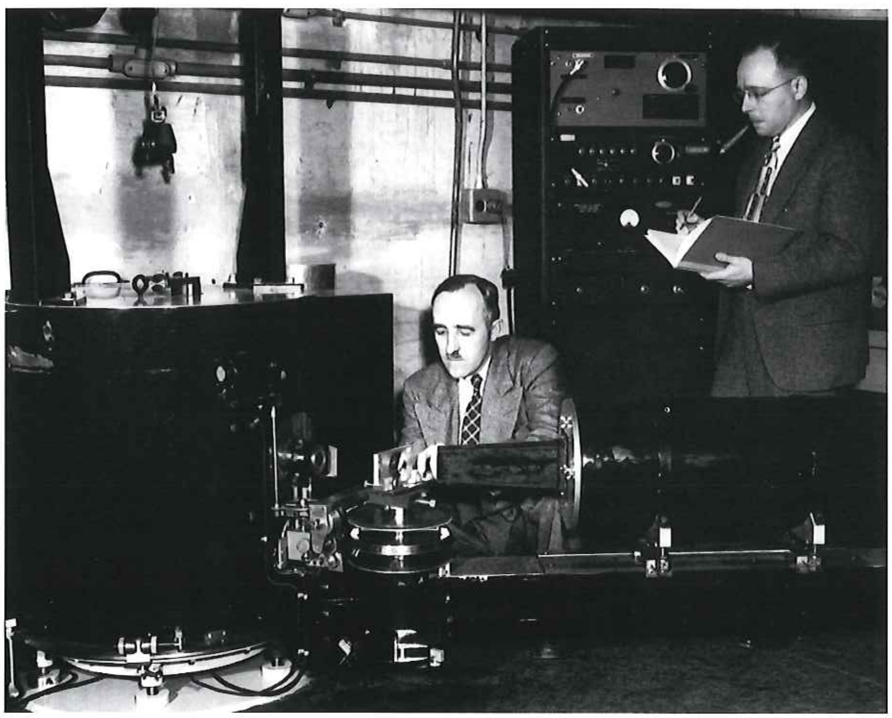
Although the United States pioneered in developing neutron sources in the 1960s, the nation has now fallen behind Europe and Japan, where a new generation of research reactors and spallation neutron sources was built in the 1970s and 1980s. The justification and need for a new neutron source in the United States has been documented by numerous scientific and government assessments since the early 1970s. The development of new instruments and measurement methods has generally increased the demand for access to neutrons.

In a 1993 study by the Department of Energy's Basic Energy Sciences Advisory Committee (BESAC) Panel on Neutron Sources for America's Future, the scientific community overwhelmingly recommended constructing a new research reactor at ORNL, the Advanced Neutron Source (ANS), for which ORNL had recently completed a thorough conceptual design.

Construction requests for the ANS were included in the President's budget for fiscal year (FY) 1994 and FY 1995, but Congress did not appropriate funds for construction of the ANS because of concern over its high cost—almost $3 billion. In the FY 1996 budget process, DOE recommended termination of the ANS, and Congress appropriated funds to begin design of a new, lower-cost spallation neutron source. In early 1996, the BESAC panel assessed the need for neutron sources and recommended

- design of a new accelerator-based spallation neutron source—namely, the National Spallation Neutron Source (NSNS) Project, and

- upgrades to the nation's high-performance research reactors, particularly the HFIR at ORNL and Brookhaven National Laboratory's High Flux Beam Reactor (HFBR), to serve researchers needing neutrons not available from a spallation source.



Cliff Shull (right), co-winner of the 1994 Nobel Prize in physics for pioneering research using neutron scattering in the 1940s and 1950s at ORNL's Graphite Reactor, performs research with Ernest Wollan at the reactor.

The NSNS will produce the highest-flux-pulsed-neutron beams in the world.

National Spallation Neutron Source

The appropriations bill passed by Congress for FY 1996 provided ORNL with $8 million to begin design of a new spallation source. The National Spallation Neutron Source collaborative project was born as ORNL's response to DOE's charge to initiate conceptual design of a new spallation source. The project is organized to take full advantage of previous studies and assessments and of technical expertise and experience at industrial firms, universities, and other DOE laboratories.

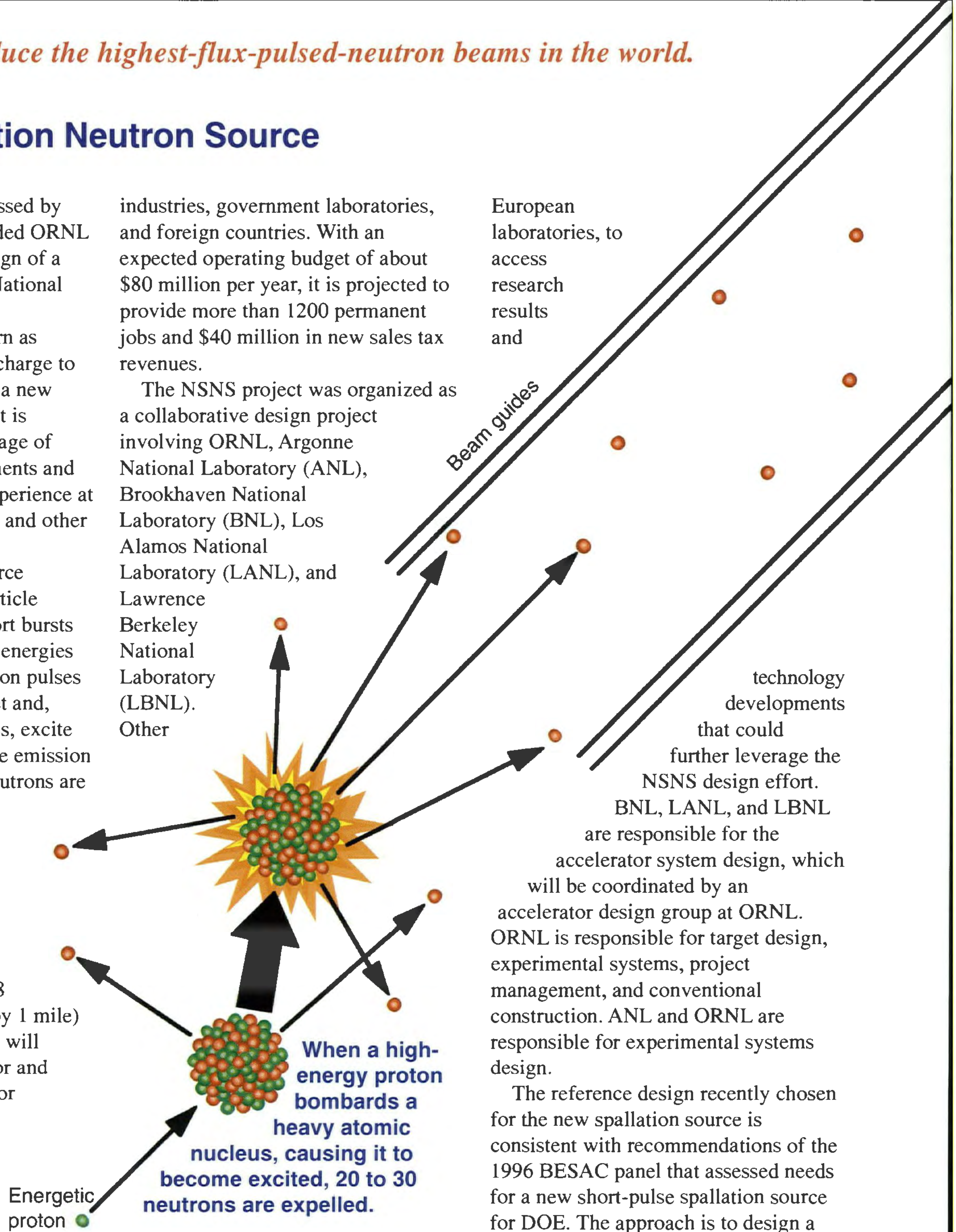
The proposed neutron source consists of a high-energy particle accelerator that produces short bursts of protons at extremely high energies and power levels. These proton pulses bombard a heavy metal target and, through the spallation process, excite atomic nuclei, resulting in the emission of neutrons. The liberated neutrons are moderated (slowed down) to useful energies and then guided as beams into experimental areas for use in neutron science experiments.

The proposed facility will occupy an area about 0.8 by 1.6 kilometers (0.5 mile by 1 mile) on the ORNL Reservation. It will consist of a proton accelerator and storage ring, target stations for production of neutrons, and experimental halls and instrumentation for use of neutrons for research and product development. The conceptual design will take two years to complete. The total cost of the facility will be about $1 billion, and it should be in operation by the year 2005.

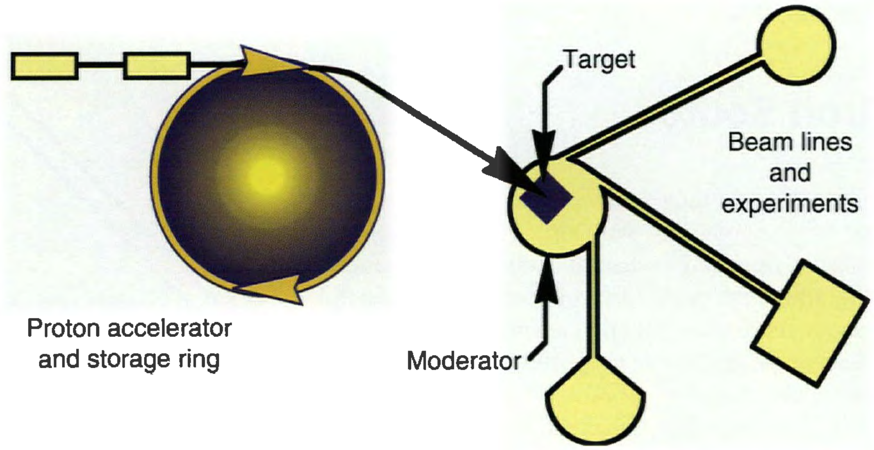
The NSNS will produce the highest-flux-pulsed-neutron beams in the world. It is estimated that the facility will attract 1000 to 2000 scientists and engineers each year from universities, industries, government laboratories, and foreign countries. With an expected operating budget of about $80 million per year, it is projected to provide more than 1200 permanent jobs and $40 million in new sales tax revenues.

The NSNS project was organized as a collaborative design project involving ORNL, Argonne National Laboratory (ANL), Brookhaven National Laboratory (BNL), Los Alamos National Laboratory (LANL), and Lawrence Berkeley National Laboratory (LBNL). Other laboratories, U.S. industrial firms, and universities will be involved as the project matures. This collaborative approach was taken to access the best technical expertise available. In addition, memoranda of understanding have been signed with the European Spallation Source—a design effort similar to NSNS—and several European laboratories, to access research results and technology developments that could further leverage the NSNS design effort. BNL, LANL, and LBNL are responsible for the accelerator system design, which will be coordinated by an accelerator design group at ORNL. ORNL is responsible for target design, experimental systems, project management, and conventional construction. ANL and ORNL are responsible for experimental systems design.

The reference design recently chosen for the new spallation source is consistent with recommendations of the 1996 BESAC panel that assessed needs for a new short-pulse spallation source for DOE. The approach is to design a 5-megawatt (MW) spallation source that can be built in stages. The first stage, which must be built for about $1 billion, will be a 1-MW source that can be upgraded to higher powers in the future, as funds allow. The 1-MW source will consist of a linac accelerator that injects negatively charged hydrogen (H^-) ions into an accumulator ring, where ~1-microsecond pulses of 1-billion-electron-volt protons are produced and



When a high-energy proton bombards a heavy atomic nucleus, causing it to become excited, 20 to 30 neutrons are expelled.



In the proposed NSNS, protons will be accelerated to high energies, formed into pulses, and directed onto a mercury target. Each pulse of protons will produce a burst of neutrons that will be moderated and guided into an experimental area.

directed to a liquid mercury target from which neutrons are generated. The target-moderator and experimental systems provide for cold and thermal neutrons servicing 18 beam lines. Several staged upgrades are possible leading to higher powers of 4 to 5 MW.

Because of the large user community expected at NSNS, ORNL, the University of Tennessee (UT), and the state of Tennessee have initiated plans for a Joint Institute for Neutron Science (JINS). This joint venture between ORNL and UT would provide meeting facilities, offices, laboratories, a communication center, and housing for scientists and engineers from universities, industries, and the international community. It would also be a focus for expanding neutron science R&D with UT, regional universities, and industrial collaborators. Funds have been included in the state of Tennessee's FY 1996 budget to begin design of JINS.

This new spallation neutron source would be the most powerful facility in the world for neutron scattering and would restore a much needed capability to the U.S. neutron science community.—*Bill Appleton, ORNL Associate Director for Advanced Materials, Physical, and Neutron Sciences.*

High Flux Isotope Reactor Upgrades

The HFIR is a multipurpose research reactor, with missions in four nationally important areas: isotope production, neutron scattering, neutron activation analysis, and irradiation testing of materials.

It was originally designed for production of the transplutonium isotopes—elements that do not occur naturally on earth and that are beyond plutonium in the periodic table of elements. One of these is californium-252, which has been used to treat more than 450 patients with advanced cervical cancers, improving the 5-year survival rate from 12% with older treatments to 54%. The HFIR remains the sole source of these isotopes in the western world and the best source of many other radioisotopes, including important medical isotopes. The HFIR's annual sales of californium-252 total about $2 million, and its radioisotopes are sold to about 800 customers a year.

Over time, neutron scattering has grown astonishingly in scientific and economic importance—providing, for example, most of our knowledge about the molecular and magnetic structure and behavior of new, high-temperature superconductors. Although the proposed package of upgrades would enhance our capabilities in all four areas mentioned above, the biggest impact would be on neutron scattering.

One part of the upgrades, a return to the original 100-MW design power level (instead of the 85 MW that has been used since 1989), will benefit all the applications discussed, because the neutron production rate, which is proportional to reactor power, will be increased by nearly 20%. Likewise, modernizing instrumentation and electrical equipment, as well as replacing certain other components of the reactor system, will reduce maintenance downtime and will increase operating time, hence more neutrons, available for all users.

For neutron scattering, there are two really major enhancements. The first is the installation of a small cold neutron source—small because there's no room for a large one—in one of the four existing beam tubes. The source will be an aluminum chamber holding about a half liter of liquid hydrogen, at a temperature of 20 K (about -420°F): at this temperature, the hydrogen molecules move fairly slowly and neutrons that enter the chamber are slowed down by collisions with those molecules. When a beam of these very slow neutrons is directed onto a sample, even very small, weak, or subtle features of atomic structure and motion can influence the speed or direction of the neutrons (as a very slowly moving golf ball is more susceptible to small irregularities or tussocks on the putting green than is a fast moving one). Thus, the more complex materials, and the weaker, more subtle forces in them, are best explored using these cold neutrons.

The best cold neutron beams in the world are those at the Institut Laue-Langevin (ILL) in France. However, because of the higher power at HFIR (100 MW vs 59 MW) and the use of new design concepts developed for the ANS, our cold beams will be brighter. Although space limitations dictate that we will have far fewer beams and instruments, the ones we do have will be the best in the world.

We propose raising HFIR's power level and adding a cold neutron source and five neutron guides.

Overview of the High Flux Isotope Reactor with proposed additions of a Thermal Guide Hall and Cold Guide Hall for providing additional beams of thermal neutrons and new beams of cold neutrons for research.

The High Flux Isotope Reactor building today. ***Photograph by Steve Eberhardt.***

The HFIR already has the world's most intense beams of thermal neutrons.

The blue glow of the HFIR fuel core submerged in cooling water.

The second change will be to put five neutron guides at an existing beam port (called HB 2) to bring neutrons from close to the reactor out into a big hall that will have space for nine experiments. Neutron guides work exactly like fiber optic guides—they are rectangular conduits, typically, 5 × 10 centimeters (2 × 4 inches), whose inside surfaces may be coated with multiple layers of nickel that will reflect any neutrons that strike the surface at a glancing angle, if they are not traveling too fast. Thus, the guides can bring neutrons from close to the reactor, in a series of ricochets, to an instrument more than 30 meters (100 feet) away, with little loss. This capability is important for two reasons: first, there isn't enough room close to the reactor for nine big instruments; second, near the reactor is considerable background radiation, including gammas and fast neutrons, that tend to swamp small signals that scientists look for. Because each guide reflects only rather slow neutrons, this undesirable background radiation escapes through guide walls, and it is absorbed by shielding before reaching the experimental sample and the detector at the far end.

The HFIR already has the world's most intense beams of thermal neutrons—those that have slowed down to the equivalent of room temperature or so. This part of the upgrade will make them brighter and purer still, as well as increasing the number of users that can be accommodated by increasing the number of beams and instruments. Office and laboratory space will also be provided for outside and ORNL researchers using the new beams.

Another important research use for the HFIR is neutron activation analysis. This very sensitive, quick technique determines elemental composition, including trace elements, in a sample. The sample is inserted in the reactor for a predetermined, usually short, time. The intense neutron bombardment will make many of the elements radioactive. The elements can be identified by detecting and measuring energies of characteristic gamma rays from the sample. A recent, important example is the analysis of samples from the floodplain of East Fork Poplar Creek in Oak Ridge for mercury, cadmium, chromium, and other environmental pollutants. Another, rather dramatic, application was the analysis of samples of hair and nails from the body of President Zachary Taylor: Almost 150 years after his death, neutron activation analysis at the HFIR showed conclusively that his arsenic levels were not elevated above normal, proving that, contrary to some historical theories, Taylor did not succumb to arsenic poisoning. The upgrade proposal includes more, and larger, facilities for accessing the reactor with samples for neutron activation and measurements on the irradiated samples.

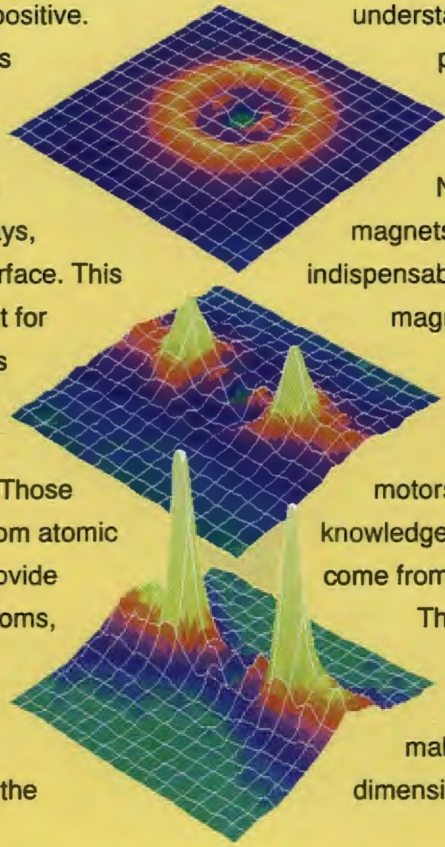
Another important research use for the HFIR is neutron activation analysis.

The development of new fusion and fission reactor systems depends on the development and testing of materials that can retain, for example, their strength, ductility, and shape, even under intense radiation. Because of its high flux and versatility, the HFIR is the preferred reactor for conducting these materials tests. The upgrade will provide improved capabilities for both handling and dismantling the test capsules.

Because neutrons are now so important to so many fields of science and engineering, the upgrade program is carefully planned to minimize the time that the HFIR will be out of service and to complete the work before the HFBR at Brookhaven shuts down for a planned upgrade of its own. The goal is to ensure that the United States will have use of one or the other of the two sources at all times.—*Colin West, manager of the Neutron Sciences Program.* ornl

Fruits of Neutron Research

Neutrons are electrically neutral, but their impact on research has been positive. Because these neutral particles interact weakly with most materials, they penetrate to great depths in a target, unlike charged particles, light, or X rays, which are stopped near the surface. This property is especially important for controlled experiments such as observing lubricant flow in an operating engine or biological molecules immersed in water. Those few neutrons that do scatter from atomic nuclei inside a material can provide unique information about its atoms, including their arrangement, motions, and vibrational energies.



Small-angle neutron scattering patterns showing the first observation of a surprising complexity in the response of a soap solution to shear flow (motion that results from spreading soap solution by rubbing hands together). As shown here, the molecular structures can become disentangled and aligned enough to flow freely.

Neutrons are used to guide the creation of new materials and new products such as Kevlar bulletproof vests and complex synthetic oils. In complex materials such as polymers and plastics that contain many atoms bound into very large molecules, a technique called molecular substitution provides unique opportunities for molecular engineering. Because neutron scattering probabilities vary substantially between isotopes such as light and heavy hydrogen (deuterium), one isotope can be selectively substituted for another within a molecule, and this tagged molecule can be observed. Such information helps researchers understand and determine the processes that produce the best plastic for a particular use.

Neutrons also behave like tiny magnets. This property has made them indispensable in the development of magnetic materials such as those used in credit cards, computer storage disks, videotapes, and electric motors. In fact, virtually all knowledge about magnetic media has come from neutron science.

The metal alloy INVAR does not expand at around room temperature. This property makes it ideal for uses requiring dimensional stability (e.g., microwave guides, lasers, metal seals, radar cavities, pressure gauges, and precision machine tools). Neutron scattering has shown that magnetic interactions of atoms in INVAR may counterbalance thermal expansion effects. This understanding opens up possibilities for new applications.

New high-temperature superconducting materials, such as yttrium-barium-copper oxides ($YBa_2Cu_3O_{7-x}$), which conduct electricity without resistance when chilled by inexpensive liquid nitrogen, may be the heart of tomorrow's energy-saving technologies. Neutron scattering has been an essential technique for understanding how the best superconducting materials are built, how they work, and how to make wires and magnets from them.

Traditional polymer processing to make new plastics creates undesirable by-products and contamination. Recently, using small-angle neutron scattering, scientists discovered new ways to synthesize polymers in environmentally safe carbon dioxide. This discovery could lead to new low-cost polymer processing techniques.

The commercial and technological success of fluids we use daily—such as lubricants, paints, and shampoos—depend largely on the ordering of their molecules under flow. For example, paint should stick generously to the brush dipped in the can but flow smoothly when brushed on the wall. This convenient property shift is caused by molecular reordering. Neutron scattering investigation of such fluids helps us understand how such reordering occurs.

Recently, researchers from Harvard Medical School and Forsyth Dental Center have jointly used neutron scattering to study interactions between collagen molecules and mineral deposits that make up the structure of bones. Neutron scattering investigations show that in healthy bones, collagen molecules form a regular nearby periodic array with an average spacing of about 1.5 nanometers, and minerals deposit in spaces along this array every 87 nanometers. Diseases like osteoporosis cause loss of mineral deposits, so adjacent spaces are no longer locked together, weakening the bones and causing them to shrink. This highly specific diagnostic tool makes it possible to devise and test remedies for demineralizing diseases.

In manufacturing processes, such as when two metal pipes are welded together or a metal part is heated, residual stresses may be trapped deep inside the metals. These stresses can cause parts to warp or break when put into use. Because neutrons can penetrate to great depths in these metal parts and "measure" variations in distances between planes of atoms compared with the normal structure, it is possible to actually map residual stresses caused by manufacturing. Such neutron residual stress measurements have been used to guide changes in manufacturing processes to produce improved automobile gears and brake rotors, welds in fuel tanks for the space shuttle, and boiler pipes in high-pressure steam generators. Penetrating neutrons could help U.S. industry penetrate new markets.

Biological Sciences

Energy heats, powers, and lights our homes and businesses, but it has a dark side. By-products of its development, production, and use can include radiation, potentially toxic chemical emissions, and greenhouse gases. For more than 50 years, ORNL researchers have studied the effects of these by-products on the health of present and future generations of living organisms. In studying biological processes, we have acquired basic knowledge that has been used in human medical treatment and in monitoring and restoring the environment.

Our investigations of the mammalian genome, especially mutations in mice, have helped scientists establish human radiation-exposure limits, find safer treatments for cancer, understand genetic disorders, and design mouse models for a variety of human diseases. Through genetic engineering, researchers are systematically manipulating (1) the genome of mice to locate genes responsible for abnormal and normal functions, and (2) protein structure of an essential life-giving plant enzyme as an avenue for increasing crop yields and decreasing atmospheric carbon dioxide, a greenhouse gas. For the future, we will focus on gaining a thorough understanding of gene-protein function in the search for medical solutions to prevent and treat disease and improve the nation's health.

Our experiment in space shows effects of no gravity on growth of nucleosome crystals.

Growing DNA-Protein Crystals in Space

On October 20, 1995, for the first time an ORNL experiment blasted off aboard the U.S. Space Shuttle Columbia, although the scheduled liftoff was September 28. The idea of the experiment was to grow near-perfect crystals of chromosome building blocks called nucleosomes by capitalizing on the absence of gravity in outer space. It is believed such crystals will grow more slowly, making them defect-free, solid instead of hollow, more uniformly shaped, and larger than nucleosome crystals grown on earth.

Because of the launch delay, most ORNL crystals had already started growing in special vials in earth's gravity. Fortunately, however, a single crystal in a highly acidic environment did not begin important growth until after the shuttle launch. Because it nucleated in space, it came back looking chunky, like a piece of thick chalk, while the other crystals resemble pencils.

The two-week experiment was regarded as a shakedown for the five-month-long crystal-growing experiments on the Russian Mir space station. These experiments were started after March 22, 1996, when the U.S. Space Shuttle Atlantis docked with the orbiting space station. From the 1995 experience the researchers learned about problems in the crystal-growing chambers, so the chambers were redesigned and new ones were built for the 1996 experiments.

Researchers from ORNL's Biology Division and other labs will peer into these near-perfect crystals using X-ray diffraction tools at ORNL and the National Synchrotron Light Source at DOE's Brookhaven National Laboratory. To protect the crystals from the damaging radiation of X rays so they may be adequately studied, ORNL researchers perfected "flash cooling," using liquid nitrogen, which works well with small crystals; they are now developing the technique to make it work for large crystals.
The goal is to obtain a detailed picture of the nucleosome's protein core and

Gerard Bunick observes nucleosome crystals in a device designed for growing crystals in space. His DNA-protein crystals were grown in zero gravity on the orbiting Russian Mir space laboratory. ***Photograph by Tom Cerniglio***

the DNA surrounding it. The nucleosome is the fundamental building block of the chromosome, a unit in a cell's nucleus that carries strands of DNA, genetic material that determines an organism's characteristics. Careful selection of the DNA base sequence in the nucleosomes allows the growth of highly ordered crystals, enabling a better view of the arrangement of atoms. The information may help scientists decipher the three-dimensional structure of a chromosome in the quest to unravel the genetic code. It is hoped that information from outer space will make understanding of earth-bound chromosomes closer to crystal clear.

Funding for this research is provided by DOE's Office of Health and Environmental Research, the National Institutes of Health, and the National Aeronautics and Space Administration.

Rescuing Mice from Kidney Disease

ORNL geneticists are on a search-and-rescue mission. They are searching for genes in mice that cause diseases like those that afflict humans. Part of their search involves rescuing the mice born with a specific disease to trace the effects of defective genes.

Take polycystic kidney disease (PKD), a condition that can cause high blood pressure, infections, and premature death in children. The genetic disease is known to cause kidney and liver lesions that are linked to localized cell proliferation. Because kidney lesions can lead to organ failure and death, children suffering from PKD are often given kidney transplants. Although kidney transplants markedly improve longevity, it's uncertain whether PKD patients might develop and die prematurely from complications associated with liver lesions.

Using genetic engineering, we produced mice born with PKD and later rescued the kidney but not the liver from the destructive effects of the disease. To produce the PKD mutation in mice, we inserted a cloned fragment of DNA into a gene to disrupt its expression. This "insertional mutagenesis" allowed us to locate, clone, and characterize the corresponding normal version of the gene that was not functioning properly in the mutant animals. Then, we reintroduced a specially modified version of the cloned gene into the mutant animals. This version rescued the kidney, but the liver lesion remained.

In the meantime, we are letting these partially cured mice age to see if they live the normal lifespan of two years. If they die prematurely, we will autopsy them to determine whether liver cancer or some other condition associated with the liver lesion eventually proves to be fatal. We will not give up the search because many are in need of rescue.

This research was supported by DOE's Office of Health and Environmental Research, Health Effects Research Program, and by the National Institutes of Health.

We produced mice with polycystic kidney disease and then saved their kidneys.

Rick Woychik (left) and Brad Yoder examine a mouse whose kidney they rescued from polycystic kidney disease. *Photograph by Tom Cerniglio.*

Mouse Mutants Important for Developing Drugs

Because mice and men possess a high degree of genetic similarity, researchers have used ORNL's unique archive of mouse strains to set radiation standards, assess health risks of chemicals, study developmental abnormalities, and clone defective genes related to human disease. Now, biotechnology firms are interested in using clonable genes from our mouse mutants to develop disease-fighting drugs. The pharmaceutical segment of the biotechnology industry is already grossing billions of dollars in sales from only a few drugs developed by the use of cloned genes.

Under a cooperative research and development agreement, we are now working with Darwin Molecular Corporation to identify mutant mice that have defective immune systems and to clone genes that are responsible for diseases. Human disorders involving malfunctioning immune systems include asthma, cancer, diabetes, multiple sclerosis, rheumatoid arthritis, and systemic lupus. Cloning genes allows us to study their function and identify the origin of immune diseases, while pharmacological manipulation of pathways from gene to disease determines strategies for immunotherapy and drug development.

Mutations are produced in mice by exposing mature male mice to radiation or a mutagenic chemical like acrylamide. The treated males are mated with untreated females. The male progeny are raised to maturity and tested for fertility. We are interested in screening the offspring of treated males that are semi-sterile, that produce half as many young as normal males. The reason: a relatively high proportion of their surviving progeny will carry observable genetic defects. Mutant mice that have immunological dysfunction will die early, develop tumors early, or have skin defects. We send tissue from these mice to Darwin.

Mutations spring from the induction of reciprocal translocations in germ cells (developmental precursors of sperm cells) of treated male mice. Translocations arise from breaks in chromosomes that lead to exchanges in and rearrangements of chromosomal parts. Because genes are located on chromosomes, genes can be broken in reciprocal translocations. When we see a mutation, disease, or defect, we suspect a broken gene. By looking at sizes and positions of stained bands of chromosomes in the light microscope, we can identify rearranged chromosomes and locate the breaks—the starting point for cloning to make copies of defective, or broken, genes. Our unique collection of clonable mouse mutants is a national treasure, and biotechnology companies are eager to help us exploit it.

Funding for our collection of mouse chromosomal mutants and research has come through DOE's Office of Health and Environmental Research and the National Institute of Environmental Health Sciences.

We identify mutant mice with defective immune systems to aid a pharmaceutical biotechnology firm.

Lisa Stubbs examines an inhabitant of ORNL's treasured Mouse House. *Photograph by Tom Cerniglio.*

Rhenium Drugs May Treat Cancer Effects

A HFIR isotope by-product may relieve cancer-induced bone pain and shrink tumors.

An agent labeled with rhenium-188 from ORNL's tungsten-188/ rhenium-188 generator shows good uptake in a patient's skeletal lesions for treatment of bone pain from metastasized prostate cancer. This study was conducted by the Nuclear Medicine Department of Kent and Canterbury Hospital in England.

In prostate, lung, and other cancers, the pain can go literally all the way to the bone. As original tumor cells spread, secondary tumors grow in the bone, causing inflammation and exerting excruciating pressure on nerves. Safe, effective, and inexpensive relief may be at hand in the form of a by-product of a tungsten radioisotope from ORNL's High Flux Isotope Reactor.

Rhenium-188, a tungsten-188 decay product that appears in ORNL-designed, soon-to-be commercialized radioisotope generators, may become the treatment of choice for cancer-induced bone pain. The energy of rhenium's beta radiation reduces inflammation and shrinks tumors, thus relieving bone pain. Rhenium can be attached to phosphorus compounds that tend to concentrate in bones.

This therapy is expected to be considerably less costly than using strontium-89, rhenium-186, and other radioisotopes currently used to treat bone pain. If studies show this prediction to be true, rhenium-188 treatment could help reduce health care costs.

In a 1995 cooperative study by nuclear medicine collaborators at Canterbury and Kent Hospital in Canterbury, England, early tests showed excellent uptake of a rhenium [Re(V)-188 DMSA] complex in skeletal lesions in patients with metastases from prostate and bronchial cancer. Because these initial studies also showed low liver and kidney uptake, therapeutic studies using larger amounts of the rhenium agent are under way to assess the agent's effectiveness in relieving cancer-induced bone pain.

Rhenium also has potential for treating other types of tumors. In a cooperative research and development agreement between ORNL and RhoMed, Inc., of Albuquerque, New Mexico, tumor-targeting agents radiolabeled with therapeutic rhenium radioisotopes are being evaluated for their effectiveness in treating tumors in research animals. The rhenium is attached to peptides, which are formed from amino acids, the building blocks of proteins. These peptides imitate the action of somatostatin, which binds to receptors on cell surfaces (somewhat like a thistle sticking to cloth). Because tumor cells also have receptors for somatostatin, peptides can be used to deliver radioisotopes to tumors like a guided missile carrying a warhead to a target.

Using rhenium-188 from the ORNL generator, RhoMed has developed a simple "kit" for on-demand labeling of its RC-160 peptide for cancer radioimmunotherapy. Peptides radiolabeled with rhenium were injected into mice having experimental tumors grown from implanted human prostate, small-cell carcinoma, and breast cancer cells. The mice were scanned to determine where the radioisotope concentrated, and results showed the tumors retained the radioactivity a long time. In addition, peptides labeled with rhenium-188 achieved a greater reduction of tumors than did rhenium-186 (produced in HFIR), demonstrating greater effectiveness of higher-energy beta particles. While no improvement was observed in untreated animals, the rhenium-188 peptide significantly shrank or eradicated tumors in treated animals.

This method offers a new approach for treatment of tumors in specific tissues, helping ORNL achieve a nuclear medicine goal. Twinkling atoms from ORNL radioisotopes may offer yet another answer to cancer.

The collaborative research with investigators at Canterbury, England, is supported by DOE's Office of Health and Environmental Research. The research with RhoMed, Inc., is supported by funds from OHER through ORNL's Small CRADA Program.

New Light on Photosynthesis

The classic theory of photosynthesis, published in dozens of textbooks, states that two structurally different components of plant membranes react with sunlight to start building plant tissue. That, however, is not the only route to photosynthesis. In studying the molecular mechanism of how green plants convert light energy into chemical energy, we found that photosynthesis can be performed with only one light reaction; two light reactions (sunlight reacting with two plant components) are not necessarily required, as the standard model predicts. When exposed to sunlight, one of these components (Photosystem II) can do it all—split water molecules to get electrons to take up airborne carbon dioxide, providing energy for plant tissue synthesis and oxygen for us. It had been thought that Photosystem I also was required to convert atmospheric carbon dioxide to plant tissue.

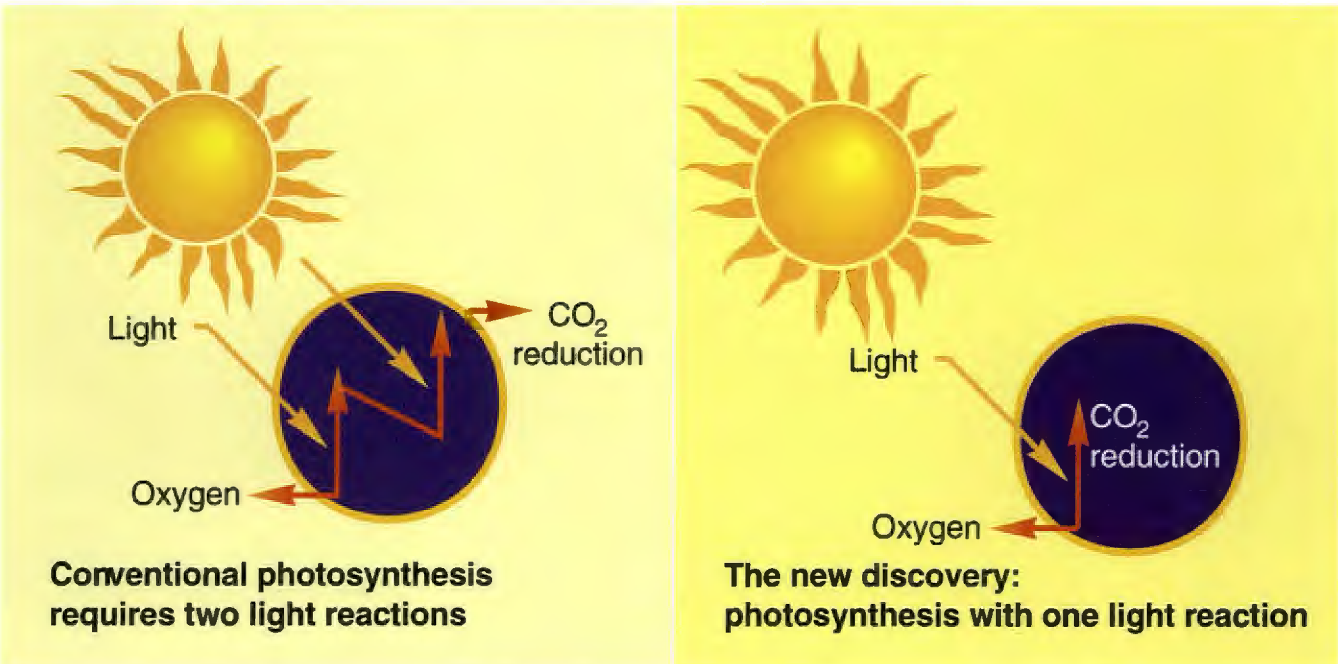
It has long been assumed that green plants evolved from photosynthetic bacteria similar to those existing today. One bacterial type, which contains iron and sulfur, is similar in structure to Photosystem I; another type, which resembles an iron-free hemoglobin, is similar to Photosystem II. But neither acts like Photosystem II, which uniquely breaks down water to produce the oxygen that sustains the animal kingdom.

However, we found that a mutant algal strain, possessing Photosystem II only, may be a model for the "missing link" of photosynthesis. At high light intensities, our mutant performs photosynthesis more stably under anaerobic conditions than in an environment containing oxygen. This is a clue to the missing link because it is generally believed that the earth's primordial atmosphere did not contain as much oxygen as today's atmosphere. One of our theories is that the hemoglobin-like group of bacteria initially developed an oxygen-producing, water-splitting capability. However, when oxygen became a major component (21%) of the earth's atmosphere by cumulative photosynthesis, this "missing" strain added a second light reaction. According to our theory, photosynthesis evolved into a two- rather than a one-light-reaction process to protect against the combined effects of high light intensities and high oxygen concentrations.

Our discovery (published in the August 3, 1995, issue of *Nature*) suggests that the maximum thermodynamic conversion efficiency of light energy into chemical energy potentially can be doubled from about 10% to 20%—a gain that could dramatically improve the productivity of food crops and biomass energy plantations, if the plants can be made to use all levels of solar energy. If that happens, the textbooks will have to be revised again.

The research was supported by DOE's Offices of Basic Energy Sciences and Energy Efficiency and Renewable Energy, the Pittsburgh Energy Technology Center, and the National Science Foundation.

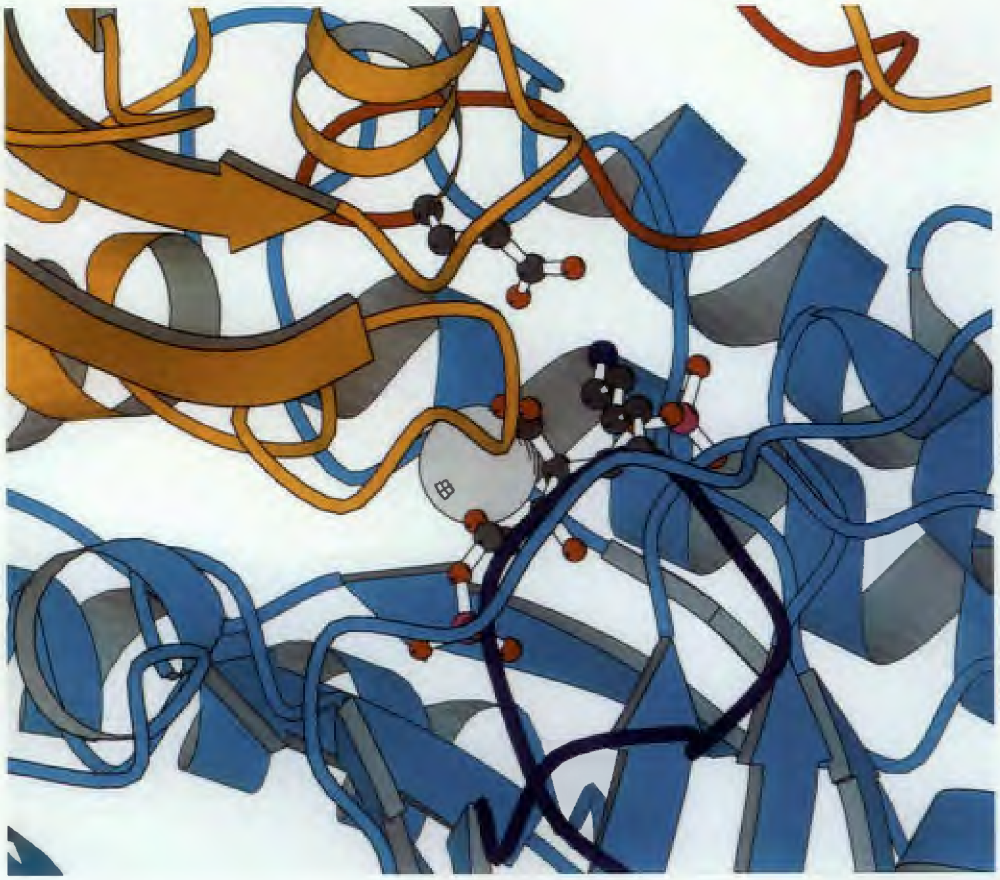
We've found a mutant algal strain that may be a model for the "missing link" of photosynthesis.



This depiction of two plant membranes (circles) shows that photosynthesis can occur with one light reaction, rather than the two explained by the classic theory of photosynthesis.

Re-engineering a Plant Enzyme

Our research shows it may be possible to tailor a key enzyme to improve efficiency of plant growth.



A key to improving the efficiency of the Rubisco plant enzyme may be to alter flexible loops in its structure (shown in this computer graphics representation) that are crucial to stabilization of reaction intermediates and their processing to normal reaction products. Models are based on atomic coordinates of the activated enzyme from tobacco (Schreuder et al., 1993, *Proc. Natl. Acad. Sci.* USA 90, 9968-9972) and are displayed using the program MOLSCRIPT (Kraulis, 1991, *J. Appl. Crystallogr.* 24, 946–950).

If the world's most abundant protein, Rubisco, could be re-engineered, growth rates of crops and forests could double, providing more food and fuel. Lush biomass would take more carbon dioxide (CO_2) from the air, controlling the greenhouse effect.

Since the 1970s, we have focused on understanding Rubisco, the CO_2-fixation enzyme present in all photosynthetic organisms. It catalyzes the initial reaction (a carboxylation) necessary to convert atmospheric CO_2 into carbohydrates and other complex biomolecules needed to sustain plant life. Unfortunately, by a quirk of nature, Rubisco can mistake the much more abundant atmospheric oxygen (O_2) for CO_2. The ensuing oxygenation reaction leads to degradation, rather than biosynthesis, of carbohydrates. As a result, energy is wasted and plant growth is restricted.

We have genetically redesigned Rubisco to learn how it distinguishes CO_2 from O_2 and how it catalyzes the two competing reactions. Our recent successes using protein engineering suggest the feasibility of altering the Rubisco enzyme to improve its efficiency.

The sequence of chemical bases in a gene instructs cells to assemble a protein from specific building blocks (20 different amino acids) in a certain order. Protein engineering involves manipulating a gene's base sequence to systematically alter a protein's amino acid sequence.

Through protein engineering, we instructed cells to produce an altered Rubisco in which one of the enzyme's 475 amino acid residues was replaced with a different amino acid. Then using protein chemistry, we modified that substitute amino acid to make it more like the original one—a modest structural change. Our tests showed that the novel Rubisco displays an altered ratio of carboxylation-oxygenation activity.

We also found a possible mechanism for crippling the enzyme's oxygen activity and enhancing its carboxylation. In many enzyme-catalyzed reactions, unstable chemical intermediates are formed along the road to final products. We identified mobile Rubisco "loops" that lock these intermediates into place so they don't decompose into nonproductive side products. If the protein's structure could be altered to selectively destabilize intermediates of oxygenation, this undesirable reaction might be undermined.

Our studies of Rubisco have greatly enhanced understanding of enzyme mechanisms in general. Because enzymes underpin all chemical reactions in all living organisms and are also the target of most therapeutic drugs, our research is benefiting society beyond the goal of attaining the biomass yield of dreams.

The research has been supported by DOE, Office of Health and Environmental Research.

We have shown that mass spectrometry is advanced enough to diagnose some diseases.

Bob Hettich and Michelle Buchanan prepare to analyze modified DNA oligomers on ORNL's 3-tesla Fourier transform ion cyclotron resonance (FTICR) mass spectrometer. A 7-tesla instrument that was to be installed in mid-1996 will substantially enhance achievable mass range and mass resolution for analysis of biomolecules. *Photograph by Curtis Boles.*

Mass Spectrometry Analyzes Biological Molecules

Once used only for lightweight, volatile molecules, mass spectrometry is becoming a heavyweight among tools that analyze bulky biological molecules. Recent revolutionary changes in technologies that introduce and sort molecules allow elucidation of the molecular weight, structural characteristics, and chemical-base sequences of heavier molecules such as DNA and proteins. ORNL has been one of the world's leaders in exploiting these remarkably flexible technologies for biological research. Through our research, we better understand how they work and how to adapt them to an ever-increasing range of analytical problems.

One new technique for introducing ions to the spectrometer is electrospray ionization (ES). It overcomes the problem of liberating nonvolatile biological molecules from solutions for study as a gas by mass spectrometry. In ES, after flowing through a thin capillary, biological molecules dissolved in a solvent are sprayed into a fine mist. These droplets are pulled through the pinhole entrance of a quadrupole ion trap mass spectrometer. There ions emerge from the droplets as naked gaseous ions that are detected. Our research showed that the ES process works like an electrochemical cell, suggesting ways to expand the ionization technique's range of applicability. Using a quadrupole ion trap, we have also developed new ways to probe the structure of trapped ES-generated gaseous biomolecules, including novel ion-ion reactions.

Another technique for generating ions from high-mass biological molecules is matrix-assisted laser desorption ionization (MALDI). Here, compounds such as DNA oligomers are mixed with a chemical (matrix) that absorbs ultraviolet laser light. In the mass spectrometer, a laser is used to vaporize the matrix molecules, which carry the ionized biomolecules into the mass analyzer.

At ORNL, two types of mass analyzers detect MALDI-generated ions—time-of-flight (TOF) and Fourier transform ion cyclotron resonance (FTICR) mass spectrometers. Our current FTICR mass spectrometer, which has a 3-tesla superconducting magnet, introduces ions at one end by MALDI and at the other by ES ionization. We are expecting delivery soon of a 7-tesla magnet, which has increased mass range and performance.

Our mass spectrometry and laser method can identify carriers of the cystic fibrosis gene.

Steve Allman (left) and Kai Tang are part of the team that developed the laser mass spectrometer for detection of genetic defects that can lead to cystic fibrosis.

We have recently developed ways to detect amplified DNA for use in molecular diagnostics. Using mass spectrometry, we have distinguished among nucleic acids of different sizes, making it an important tool in diagnosing disease, analyzing bacteria in the environment, screening consumer products for contamination, and characterizing evidence that could be used in court.

Using MALDI TOF, we have identified a segment of DNA that is specific for the bacterium that causes Legionnaire's disease. We have also developed the capability to detect DNA fragments with a three-base deletion, characteristic of individuals who have cystic fibrosis. Evaluation of this capability has shown it can be used to screen individuals for cystic fibrosis.

We continue to explore new ways to detect and structurally analyze smaller quantities of biological molecules at higher sensitivities, while minimizing the need for extensive sample preparation. With these advances, mass spectrometry is emerging as a standout among tools for analyzing complex biological molecules.

DOE's Offices of Basic Energy Sciences and Health and Environmental Research and ORNL's Laboratory Directed Research and Development Fund supported this work.

New Technique for Cystic Fibrosis Gene Screening

Cystic fibrosis (CF) is an inherited, fatal disease in which mucus buildup promotes digestive disorders and bacterial infections in the lungs. CF patients must take heavy doses of antibiotics and often die young.

Because each person with CF is the child of parents who both carry defective forms (alleles) of a particular gene, there is interest in large-scale screening to let people know their chances of having a child with CF.

We have developed a new technique that could be used to rapidly screen many people for a specific defect in a gene on chromosome 7 that causes 70% of all CF cases. The defect is the absence of three base pairs of DNA in both alleleles that control production of CFTR, a protein that prevents mucus buildup. CF carriers have a single defective allele that may be passed on to their offspring. CF patients have two defective alleles.

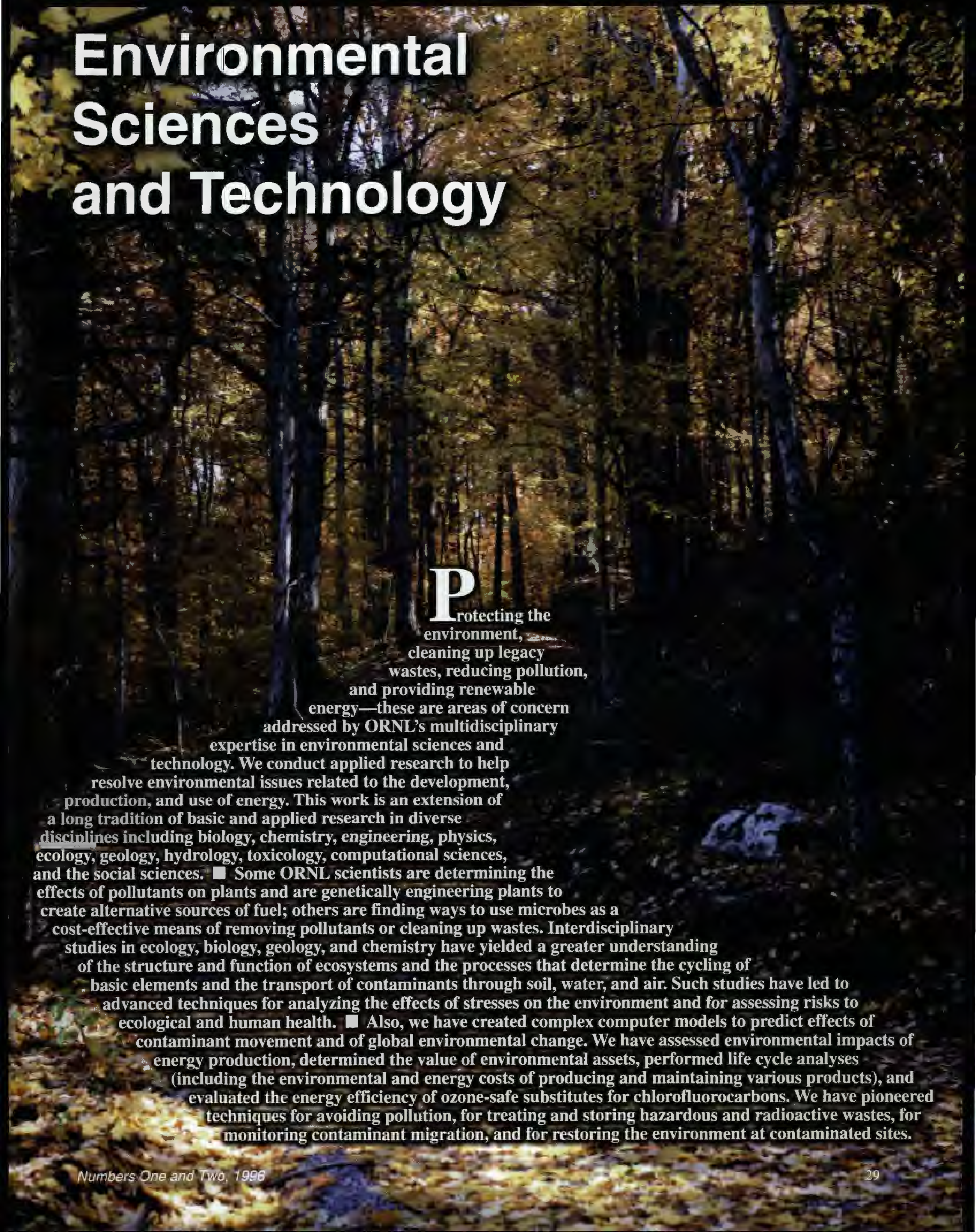
Our CF gene screening technique uses laser mass spectrometry, marking the first time that mass spectometry has been used to diagnose a genetic disease by DNA analysis. The technique screens in minutes, not hours, making it ten times faster than conventional gel electrophoresis. Also, it does not use toxic chemical or radioactive materials, which require costly methods of disposal.

For the experiment, researchers from ORNL and the University of Tennessee Medical Center (UTMC) extracted DNA from human hair samples and isolated and copied millions of times the part of each CF gene that would contain the known defect if present.

After receiving 30 droplet samples for a blind test, the researchers mixed each DNA segment with a chemical that absorbs ultraviolet laser light and vaporized the mixture with a laser. The electrically charged DNA segments formed in the vapor were separated by size in a time-of-flight mass spectrometer; the defective alleles that lack three DNA base pairs are smaller and lighter and, therefore, travel faster than the heavier, normal gene segments. ORNL's identifications of the 30 samples agreed completely with the results of conventional analyses, showing the technique was 100% accurate in distinguishing between normal and defective CF genes.

The research was supported by ORNL's Laboratory Directed Research & Development Fund and by DOE's Office of Health and Environmental Research. **ornl**

Environmental Sciences and Technology



Protecting the environment, cleaning up legacy wastes, reducing pollution, and providing renewable energy—these are areas of concern addressed by ORNL's multidisciplinary expertise in environmental sciences and technology. We conduct applied research to help resolve environmental issues related to the development, production, and use of energy. This work is an extension of a long tradition of basic and applied research in diverse disciplines including biology, chemistry, engineering, physics, ecology, geology, hydrology, toxicology, computational sciences, and the social sciences. ■ Some ORNL scientists are determining the effects of pollutants on plants and are genetically engineering plants to create alternative sources of fuel; others are finding ways to use microbes as a cost-effective means of removing pollutants or cleaning up wastes. Interdisciplinary studies in ecology, biology, geology, and chemistry have yielded a greater understanding of the structure and function of ecosystems and the processes that determine the cycling of basic elements and the transport of contaminants through soil, water, and air. Such studies have led to advanced techniques for analyzing the effects of stresses on the environment and for assessing risks to ecological and human health. ■ Also, we have created complex computer models to predict effects of contaminant movement and of global environmental change. We have assessed environmental impacts of energy production, determined the value of environmental assets, performed life cycle analyses (including the environmental and energy costs of producing and maintaining various products), and evaluated the energy efficiency of ozone-safe substitutes for chlorofluorocarbons. We have pioneered techniques for avoiding pollution, for treating and storing hazardous and radioactive wastes, for monitoring contaminant migration, and for restoring the environment at contaminated sites.

Ozone, Climate Change May Slow Tree Growth

Without air, plants could not live. But air also carries pollutants from natural processes, fossil-fuel power plants, and highway vehicles that can endanger tree health. Among these pollutants are ground-level ozone, which forms when airborne hydrocarbons and nitrogen oxides react in sunlight, and greenhouse gases, which threaten to alter climate.

ORNL scientists have found that ground-level ozone in the environment can reduce the growth of the loblolly pine, a forest tree species of economic importance in the Southeast. Their findings, reported in March 1995 issues of the journal *Nature* and *The New York Times*, suggest that forest tree growth could significantly decline because of exposure to ozone combined with the higher temperatures and increased drought predicted as a part of our future global climate.

In the 1980s, reductions in growth of loblolly pine trees in the Southeast were observed. This decrease aroused concern because loblolly pine is an important component of southern pine forests. Logging of southern pine forests, which cover an estimated 60 million acres, contributes over $4.5 billion annually to the regional economy.

Studies of tree seedlings exposed to ozone in closed chambers at ORNL and elsewhere showed the pollutant stunted seedling growth. The new ORNL study, which precisely measured growth patterns of tree trunks of mature trees and used statistical techniques to separate ozone effects from other influences, is the first to determine that ozone retards mature tree growth in a real forest environment.

Under normal ozone levels in the eastern United States, we observed tree growth reductions of 5%, except during the wettest years. The decline was more pronounced under dryer conditions (up to 13%). When ozone levels were especially high, tree trunks actually contracted slightly during the driest periods.

Evidence from other studies suggests that ozone may impair a tree's ability to efficiently use available water. How? By increasing water losses through foliage and reducing root growth, thereby lowering water uptake. Thus, ozone can magnify effects of water stress on tree growth.

Sandy McLaughlin (left) and Darrell Downing precisely measure the growth of loblolly pine trees in a forest exposed to high ozone levels and hot, dry conditions. Inset: Growth of each tree was monitored by a dendrometer, a metal band positioned around the trunk that precisely measures fluctuations in its expansion rate. *Photograph by Tom Cerniglio.*

When it's hot and dry and ozone is high, loblolly pine growth is stunted.

Some computer models predict that future climate change will be marked by increasing temperatures and drought. Our results suggest that trees exposed to ozone under these climatic conditions would experience significant reductions in growth. Even for trees, change is in the air.

Funding for this research was provided by the U.S. Forest Service Global Change Program.

Trees Emit Mercury

Like most people, some green plants like to give as well as receive. In the 1970s, we discovered that plants can take up mercury from soil and air. Now, 20 years later, we have scientific proof that plants emit mercury to the air.

This finding came from an ORNL-designed study in the laboratory and field. We sought to determine if the landscape mainly emits mercury to the air or if it stores mercury deposited on it from air. In this study, a high-precision sampling technique developed at ORNL measured exchanges of mercury between air and land to see if land is a mercury source or sink.

In laboratory experiments, maple, oak, and spruce saplings were grown in a chamber into which low-mercury air was introduced. The soil the saplings were planted in was isolated from the chamber. When a researcher sampled the air for mercury vapor, he was surprised that mercury was coming from the plants.

Further experiments showed that the plants take mercury from the air when the air's mercury level is above about 20 nanograms per cubic meter. When the mercury level in air is only

Under certain conditions, green plants return stored mercury to the air.

2 nanograms per cubic meter, the plants emit mercury. These different levels of mercury occur near pollution sources and at background sites respectively.

We also measured gradients in mercury concentrations over Tennessee forests. Meteorological tower data from Walker Branch Watershed in Oak Ridge showed significant emissions of mercury from oak, hickory, and maple trees below. Our studies of trees at a Christmas tree farm in Wartburg showed that mercury deposits from air to trees when they are wet. We also observed that trees there are a strong source of mercury to the air when they are dry, supporting data from our laboratory studies.

ORNL researchers theorize that elemental mercury in soil gas is pulled into the plant when the plant's mercury level is low. The plant tries to achieve equilibrium with respect to mercury levels in the air. When the plant's mercury level rises and the air mercury level decreases, at some point the plant releases some of its mercury to the air. Some mercury-containing plants are waiting to exhale.

This research was sponsored by the Electric Power Research Institute, the research arm of the U.S. electric utility industry.

Newly Discovered Bacteria Produce Magnetic Material

In 1993, while Texaco engineers explored for oil and gas deposits near the Chesapeake Bay, ORNL microbiologists working in a trailer by the oil company's derrick discovered novel bacteria. Studying samples extracted by Texaco from a depth of 2800 meters (91,000 feet), the microbiologists observed that metallic compounds had been chemically altered by microbes at a temperature of 70°C (158°F), even though the subsurface samples had been geologically isolated for some 100 to 140 million years.

In 1994 ORNL researchers determined that these microbes from the Taylorsville Triassic Rift Basin near Fredericksburg, Virginia, have an interesting capability: they produce magnetic material. The researchers isolated micron-size bacteria and found that these microorganisms produced nanometer-scale magnetic iron precipitates. The researchers also found evidence that the microbes can remediate groundwater containing chlorocarbon compounds (trichloroethylene and tetrachloroethylene) and heavy metals.

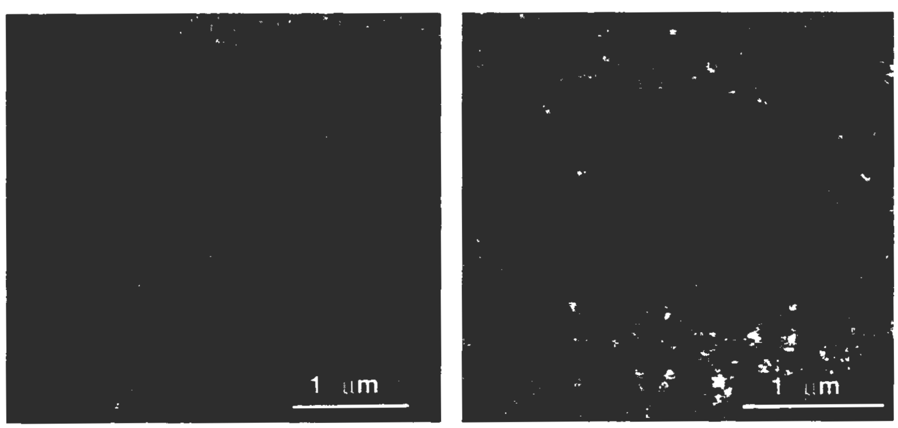
The researchers found similar bacteria at the Naval Oil Shale Reserve at the Piceance Basin in Colorado. Both the Taylorsville and Piceance basins, although separated geographically and formed at different times, contain deep subsurface formations heated by compression to high temperatures. The thermophilic (heat-loving) bacteria feed on compounds containing carbon, hydrogen, and oxygen, such as acetate and lactate (an ingredient of sour milk). The Piceance Basin bacteria, which also metabolize hydrogen and pyruvate, were found in groundwater and drilling mud; the Taylorsville bacteria were present in subsurface shale and sandstones.

The anaerobic bacteria convert food to energy and waste through an electron transfer process typical of respiration, rather than fermentation. Just as humans get rid of electrons by forming and exhaling carbon dioxide, these bacteria dump electrons on nearby electron-accepting metals, such as iron. In the process, they reduce iron hydroxide [$Fe(OH_3)$] to magnetic iron (Fe_3O_4). These magnetite particles can catalyze the degradation of chlorocarbon compounds. The bacteria can also reduce other electron-accepting heavy metals such as chromium, cobalt, and uranium, making the bacteria potentially useful for bioremediation of soil and groundwater contaminated with mixed waste, if the environment is sufficiently heated.

Potential biotechnological applications of these bacteria include the production of magnetic fluids for brakes and lubricants for high-speed turbines. The bacteria also are of interest to researchers studying the evolution of the atmosphere, the banded iron formations responsible for the earth's magnetic field, and respiration in organisms. With these bacteria, we can look back to steps of natural evolution or ahead to progress in the biotechnology revolution.

The research was supported by DOE, Office of Health and Environmental Research.

We identified subsurface microbes that could remove heavy metals from soils and groundwater.



Living on hydrogen in drilling mud, these newly discovered bacteria produce tiny particles of magnetic iron oxides, as shown under a scanning electron microscope.

Guy Griffin (left) and Paul Gailey use a fluxgate magnetometer to perform a calibration check of ORNL's magnetic field exposure system, which exposes biological cell cultures to precise magnetic fields in an environment in which temperature, humidity, and carbon dioxide are controlled. Cell cultures are placed in two chambers, but the control electronics turn on exposure fields in only one (and the researchers don't know which one, ensuring that no inadvertent bias enters the experiments). ***Photograph by Tom Cerniglio.***

Electromagnetic Fields and Body Cells

Some people have a fear of fields—electromagnetic fields (EMFs) from power lines and electric blankets. They are concerned about evidence suggesting that EMFs cause leukemia and brain cancers. Because of their health concerns and the associated economic impact (e.g., inability to site new lines, re-engineered appliances, and the expense of underground siting of power lines), the Energy Policy Act of 1992 has authorized government researchers to find out if these fears are grounded in science.

Since 1990, ORNL has played a major role in the national EMF research effort, and in 1995, it became one of four government facilities charged with determining whether published results of several EMF experiments can be replicated under controlled conditions. Here are some recent scientific scenes at our Electromagnetic Fields Bioeffects Laboratory.

ORNL scientists obtain some genetically engineered breast cells from a researcher in France. When properly cultured, these cells are designed to give off faint but detectable light when exposed to estrogen or estrogenlike compounds such as DDT. Exposure of these cells to estrogen shows at least one gene expresses itself (causes itself to produce effects), as revealed by light emission. We are studying the effects of EMFs on these cells to see if the genetic region sensitive to estrogen also responds to EMFs of certain strengths by emitting light.

ORNL has one of four U.S. Electromagnetic Fields Bioeffects laboratories.

A technician removes cells from a 6-day-old fertilized egg that would eventually form a chick's heart. The beating rate of the throbbing heart cells is measured by an ultrasensitive pressure transducer, a sort of miniature stethoscope. The heartbeat is slightly irregular, which is normal. Scientists then expose the heart cells to electric fields like those induced in the body by exposure to moderately strong EMFs. They discover that certain electric fields perturb the heart cells, increasing or decreasing their beating rate in regular synchrony with the field's frequency. More experiments will help determine how low an electromagnetic field must be before the heart cells show no signs of perturbation.

An ORNL scientist uses this information in his mathematical models to predict the weakest electromagnetic fields that cause perturbations and other bioeffects in specific cells. These fields will then be compared with EMFs to which the public is exposed. For some scientists, the study of EMF bioeffects could be a field of dreams.

EMF bioeffects studies at ORNL were initiated through a grant from the Laboratory Directed Research and Development Program and are now supported by DOE's Office of Energy Management.

Helping the Army Assess Disposal of Chemical Weapons

We've helped the Army prepare an environmental impact statement for a proposed munitions incineration facility.

Chemical weapons were made to kill, so few Americans want to keep them around. Taking orders from Congress and heeding international disarmament treaties, the U.S. Army has been seeking the safest way to destroy our nation's stockpile of toxic munitions. Stored in reinforced concrete igloos, these weapons comprise 3.3 million rockets, artillery shells, bombs, and land mines filled with nerve gas and blister agents.

In the mid-1980s, the Army faced a dilemma. It had decided to destroy the obsolete chemical weapons stored at eight depots, but it wanted to minimize the risks. Should it ship the weapons to one central disposal location or dispose of them at each of the storage sites? The Army turned to ORNL to assess the environmental impacts of the disposal options. Our team of environmental, health, and transportation specialists showed the Army that it would be far safer and environmentally preferable to destroy the weapons on-site than risk transportation accidents.

In the early 1990s, after deciding to destroy the munitions by incineration, the Army asked our help in preparing a site-specific environmental impact statement for a proposed chemical weapons incineration facility at the Pine Bluff Arsenal in Arkansas. So, using a variety of computer techniques, we determined the potential environmental and socioeconomic impacts of constructing and operating a facility for destroying the arsenal's inventory of chemical weapons. We used geographic information system software for evaluating issues of environmental justice—for example, are minority and low-income populations in the vicinity of the depot more likely to be affected by potential incineration emissions? The potential consequences of an unlikely hypothetical accident were found to be up to 4200 deaths for the worst-case scenario.

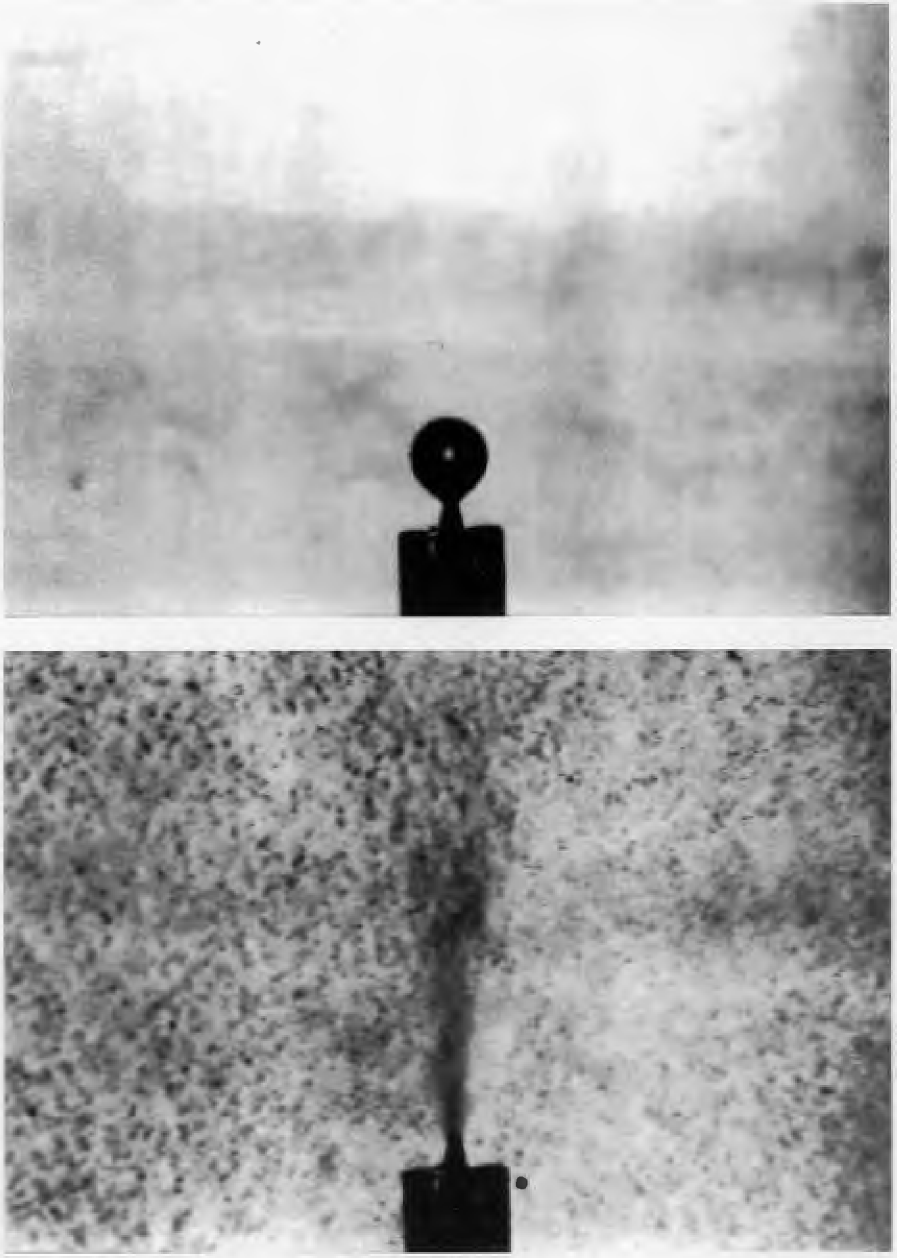
For comparison, we assessed the potential impacts of continued storage of the arsenal's inventory (one problem is that chemicals could corrode casings and leak out into the igloos). The Army released our draft document for comment on June 9, 1995; the final impact statement is being completed, taking into account the comments received.

Construction of the disposal facility is scheduled to begin in late 1996. During operations, the munitions containing the chemicals will be loaded onto conveyor belts and disassembled by remote-controlled machines. Then the chemical agents, munition parts, and explosive components will be incinerated. Destruction of the arsenal's inventory of 3850 tons, or 12% of the total U.S. chemical weapons stockpile, is expected to begin in late 1999. After an estimated 38 months of operation, the disposal facility will be dismantled and closed. And by 2004 it is hoped the Army's book on U.S. chemical weapons will also be closed.

Obsolete chemical weapons in storage at a U.S. Army depot.

Applying Inverse Electrostatic Spraying

We have demonstrated and explained inverse electrostatic spraying, which could cleanse polluted water.



ORNL has demonstrated electrostatic dispersion of nonconductive fluids into conductive fluids, as shown here. Results could lead to effective nozzle design for cleansing polluted liquids.

In 1750, French cleric and physicist Jean-Antoine Nollet demonstrated that water dripping or flowing from a vessel would form an aerosol if the vessel were electrified and placed near a ground. Nollet noted that any electrically conductive fluid would behave the same way when passing into a nonconductive medium under similar conditions. He pointed out that, for example, "a person, electrified by connection to a high-voltage generator, would not bleed normally if he were to cut himself; blood would spray from the wound." A woodcut portrayal of a man in such a ghastly predicament appears in Diderot's encyclopedia.

Since Nollet first observed electrostatic spraying, it has become a useful tool for consumers and for industry. Electrostatic spraying is the principle behind inkjet printing. It also makes car spray-painting and crop spraying more efficient in two ways. Large drops are broken into a fine mist, providing a more uniform coating, and the particles are attracted to a grounded auto body (or a fruit tree grounded by its roots), resulting in less waste and less pollution.

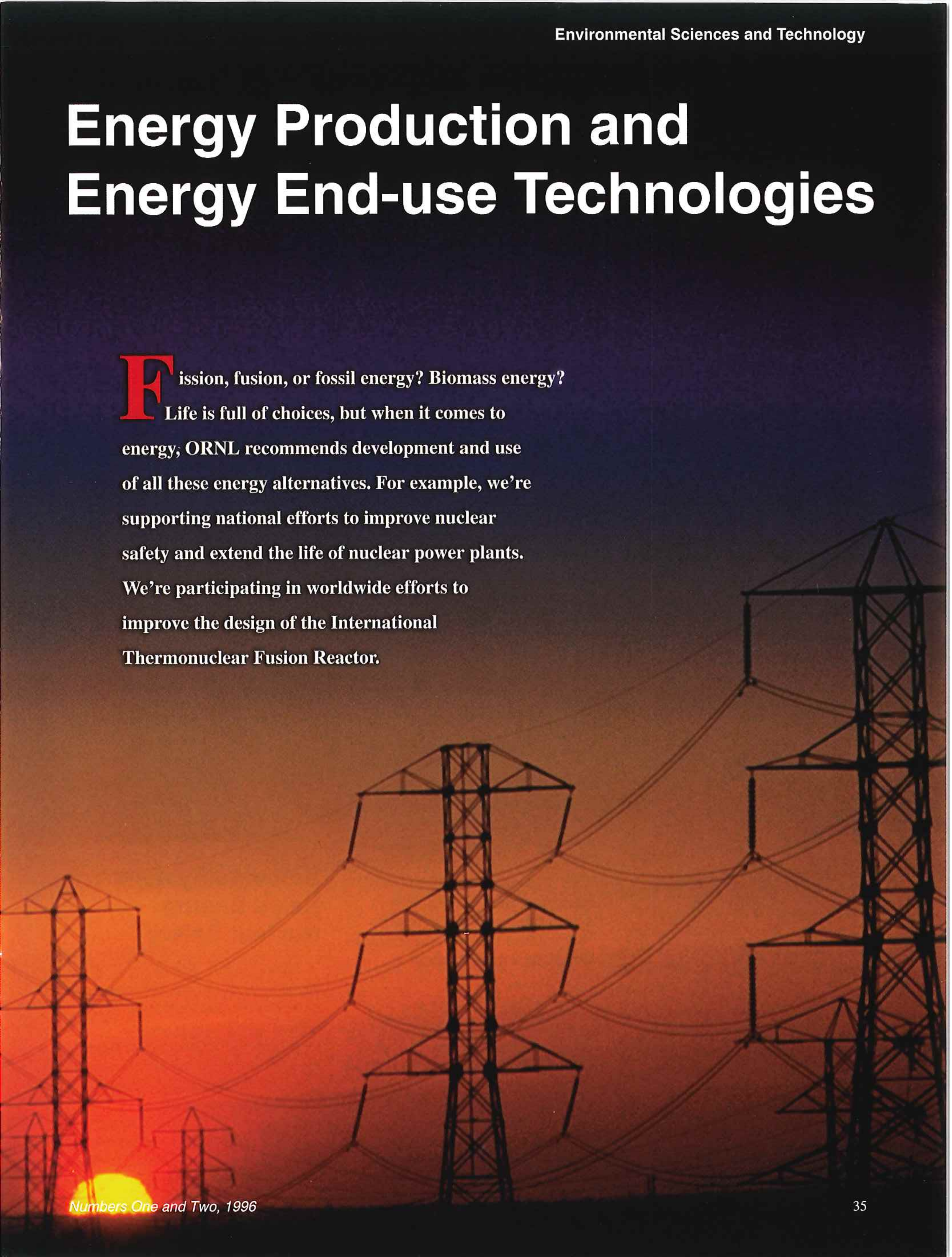
Recently, researchers at ORNL have applied the same principles to mixing liquids that would otherwise not combine, permitting efficient chemical processes that would otherwise be difficult or impossible. Examples are the emulsion-phase contactor for liquid extraction and the electric dispersion reactor for materials synthesis.

It was long thought that reversing this process, spraying a nonconducting fluid into a conductor, was impossible. Recently, however, inverse electrostatic spraying has been demonstrated and its mechanism has been explained at ORNL. This phenomenon may prove useful for waste management and environmental restoration.

For example, a gas pumped into polluted water can collect and remove harmful chemicals, or "scrub" the water. By breaking large bubbles into many small bubbles, inverse electrostatic spraying boosts the efficiency of this process in two ways. It increases the contact time of the gas in the fluid (small bubbles move slower than large bubbles), and it increases the surface area, creating more opportunity for the pollutants to migrate to the gas. In a similar way, a reactive gas, such as ozone, can break down harmful chemicals into harmless components while killing bacteria. In nearly 250 years, the world has come a long way in learning how to spray.

Funding for this research has been provided by DOE, Office of Energy Research, Basic Energy Sciences, Division of Chemical Sciences. **ornl**

Energy Production and Energy End-use Technologies



Fission, fusion, or fossil energy? Biomass energy? Life is full of choices, but when it comes to energy, ORNL recommends development and use of all these energy alternatives. For example, we're supporting national efforts to improve nuclear safety and extend the life of nuclear power plants. We're participating in worldwide efforts to improve the design of the International Thermonuclear Fusion Reactor.

We're also investigating and promoting ways to save energy in the home, office, and factory. Recently, we've created a new high-temperature superconducting wire, a converter that could cut costs of high-voltage direct-current power transmission, a procedure to help users measure R-value in walls, and a computer model that predicts energy losses from wall-floor connections, or thermal shorts.

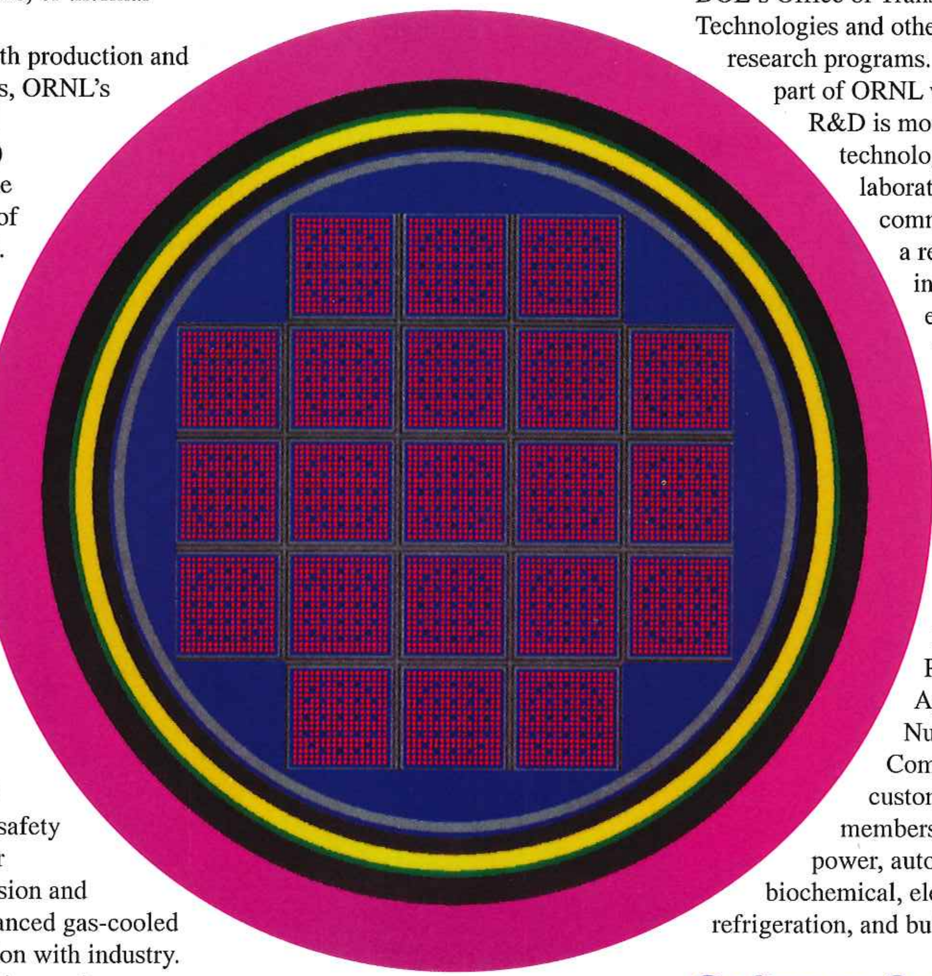
Encompassing both production and end-use technologies, ORNL's energy research and development (R&D) program is one of the premier enterprises of its kind in the world. Its strong applied focus is underpinned by fundamental investigations in the basic energy sciences and by the integration of many diverse technical skills.

Energy-production R&D is one of ORNL's oldest programs, dating back to the mid-1940s. Today, fission reactor R&D emphasizes nuclear safety work for the Nuclear Regulatory Commission and development of advanced gas-cooled reactors in cooperation with industry. Fusion energy R&D is a major component of DOE's Magnetic Fusion Program and involves collaboration with other research institutions, both nationally and internationally. Biomass energy R&D includes both conversion to end-use fuels and energy crops, with ORNL serving as technical manager for the national program on energy crop development. Fossil energy R&D includes materials research, coal combustion, and bioprocessing.

End-use technologies cover a wide range of applications for buildings, industries, and transportation. An important component of the buildings R&D program, which includes both thermal envelopes and equipment, is the Buildings Technology Center, a user facility for testing elements of buildings and equipment. Our contributions include advanced air conditioning and refrigeration systems and testing of insulation and roof systems. Industrial energy efficiency R&D focuses on advanced materials for heat exchangers and other industrial uses, advanced bioprocessing concepts, industrial gas turbines, and alternative chemical feedstocks. Transportation R&D involves materials, propulsion technologies, alternative fuels, transportation data, and policy analysis.

The High Temperature Materials Laboratory, another user facility, houses several laboratories to support DOE's Office of Transportation Technologies and other DOE materials research programs. A significant part of ORNL work on energy R&D is moving technologies from the laboratory to the commercial sector. As a result, industry is involved in almost every energy technology program. In addition to such major federal clients as DOE, the Department of Transportation, the Environmental Protection Agency, and the Nuclear Regulatory Commission, customers include members of the nuclear power, automotive, biochemical, electric utility, refrigeration, and building industries.

ORNL's popular SCALE software can tell how much spent fuel can be safely loaded into transport casks.



This geometric model of a transport cask loaded with assemblies of spent nuclear reactor fuel is a visualization of the SCALE code system.

Software System Helps Ensure Nuclear Safety

Engineers and scientists involved in the fabrication, storage, and transport of nuclear fuel used in reactors must address nuclear safety concerns. Is there sufficient shielding surrounding the spent fuel to protect people from radiation? Will spent fuel storage or transport casks stay within a temperature limit and avoid rupture under internal heating from nuclear fuel or external heating from fires in hypothetical accidents? Is the facility or cask design sufficient to prevent a criticality incident involving an uncontrolled release of energy and radiation?

To analyze various accident scenarios accurately and comply with safety regulations of agencies such as the U.S. Nuclear Regulatory Commission (NRC) and the International Atomic Energy Agency, people throughout the world use ORNL's popular Standardized Computer Analysis for Licensing Evaluation (SCALE) code system. Over the past decade SCALE has been used to analyze the disassembly and shipment of the damaged Three Mile Island reactor and the transport of highly enriched uranium from Kazakhstan to the Oak Ridge Y-12 Plant storage facility for Project Sapphire.

In 1995, to improve users' abilities to evaluate safety concerns, SCALE Version 4.3 was completed, tested, and released for public distribution. This modular, versatile version of SCALE offers automated data processing and computer modeling to predict the composition of spent fuel from a reactor and determine the distribution of radiation and heat in a cask. Among its improvements are visualization capabilities (color graphics of model geometries) and simple procedures for installation on a variety of workstations and personal computers. We have trained people throughout the United States, Europe, and Asia in how to use SCALE, and it has been important in ORNL collaborations with Japan, Germany, Italy, Thailand, the Netherlands, the United Kingdom, and the Ukraine.

When nuclear fuel is burned in a reactor, its composition changes, reducing its ability to achieve a critical configuration. Traditionally, criticality safety assessments have not taken credit for these reductions. If "burnup credit" can be accurately considered in safety analyses, more spent fuel could be safely loaded into storage and transport casks. ORNL and Sandia National Laboratories provided technical underpinnings for such a recommendation, which was submitted by DOE to the NRC in June 1995. SCALE has been used to weigh in on physics and analysis issues linked to burnup credit. If burnup credit is allowed, far fewer shipments would be needed to move spent fuel from reactors to a final disposal site, reducing the risk of a transportation accident and costs of spent fuel disposition.

The development and maintenance of SCALE is sponsored by the NRC and DOE's Office of Environment, Safety and Health. The work to investigate technical issues related to burnup credit is sponsored by DOE's Office of Civilian Radioactive Waste Management.

ORNL Assessing Annealing of Reactor Pressure Vessels

Heat could be a key to the future of the nuclear power industry. Nuclear energy, of course, provides heat that is converted to electrical power. But uncontrolled heat generation could lead to costly power plant shutdowns. Controlled use of heat could extend the life of reactor pressure vessels.

Here's the problem. Aging nuclear-reactor pressure vessels, especially those containing nickel alloys and copper impurities, may become embrittled by neutrons from the fissioning fuel core. If the hot vessel walls ever become too brittle and are chilled by cold water injected to replace the accidentally lost pressurized coolant (pressurized thermal shock), cracks could develop because of the vessel's reduced fracture toughness. The water that cools the fuel could then leak out, causing the fuel to overheat and melt portions of the vessel wall, releasing radioactivity to the containment building.

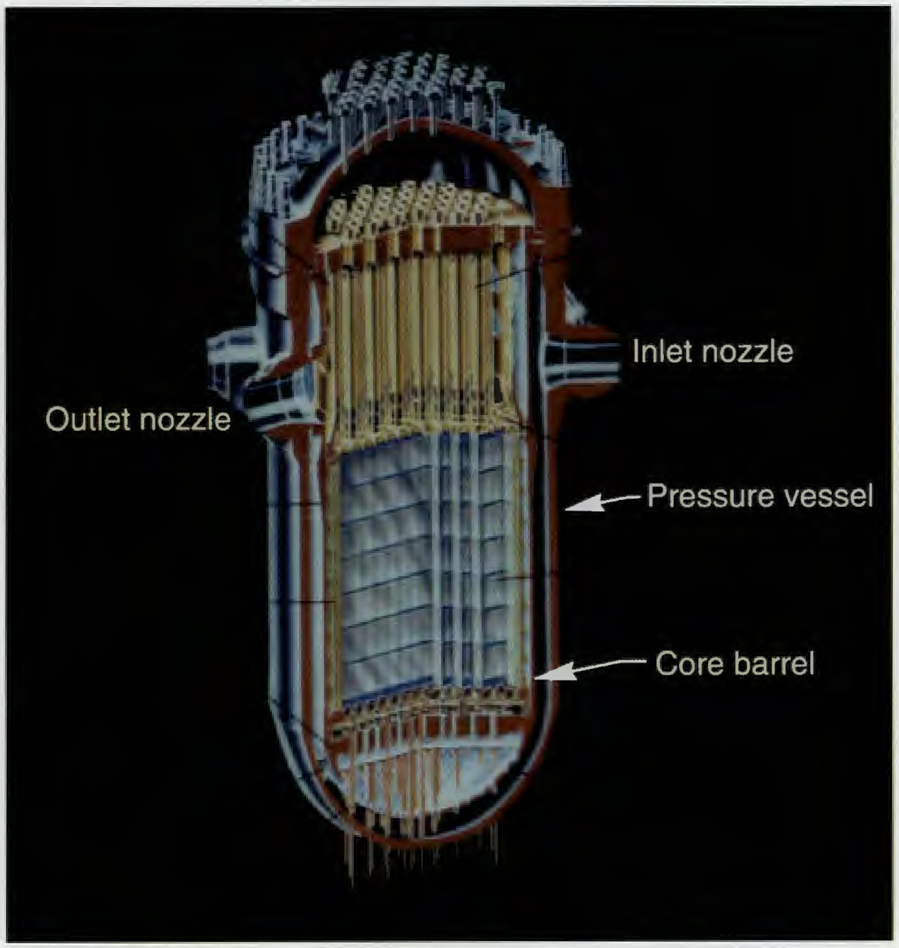
Here's a possible solution—thermal annealing. In Russia, embrittled vessels have been emptied of water and heated electrically to about 454°C (850°F) for about a week. This thermal annealing process has restored ductility to the vessels. The theory is that vessel walls will remain ductile if atoms dislocated by neutron irradiation are free to move around. But if clusters of displaced atoms and resulting voids (point defects) and copper-rich precipitates block the motion of dislocations, the material becomes brittle. In thermal annealing, the heat tends to dissipate the defect clusters and coarsen the copper-rich precipitates, greatly decreasing their number density. As obstacles to dislocation motion fall, fracture toughness and ductility are recovered in the vessel wall.

American reactor pressure vessels differ from Russian ones in that their welds run in both longitudinal and circumferential directions (a typical Russian vessel has only a circumferential weld). As a result, thermal annealing could introduce potentially damaging temperature gradients in the vessel's nozzle region where water enters and leaves. If the vessel expands in this region near a weld, the stresses might damage pipes and adjacent components.

To determine whether thermal annealing is safe and effective for U.S. reactor vessels, DOE's Light Water Reactor Technology Center at Sandia National Laboratories is demonstrating annealing on unirradiated pressure vessels at the abandoned Marble Hill and Midland-2 nuclear power plants near Louisville and Detroit respectively. The NRC has asked ORNL to help it evaluate these demonstrations and the engineering feasibility of annealing U.S. reactor pressure vessels.

ORNL researchers are conducting thermal and stress analyses of the annealing process to assess the adequacy of the annealing vendor's instrumentation plan. The vendor's instruments should (1) verify that the required annealing temperature has been achieved and maintained for the required time and (2) provide data that can be used to confirm that components and structures on or near the vessel were not damaged during annealing.

We're helping the NRC determine whether thermal annealing is safe and effective for U.S. reactor vessels.



To maintain the ability to cool the fuel core of a nuclear reactor, integrity of the reactor pressure vessel must be preserved. To prevent fracture of the vessel, irradiation damage levels must be limited in the belt-line region below the inlet and outlet nozzles. As the vessel ages, it may be necessary to alleviate radiation damage in this region by thermal annealing.

The results from this project are expected to assist the NRC in evaluating the adequacy of the operating plan called for in its thermal annealing rule and regulatory guide. The plan requires an evaluation and demonstration that the reactor's operability will not be detrimentally affected by thermal annealing. It is hoped that when the project is completed in June 1997, the evaluation will shed more light than heat on the issue of whether annealing is appropriate for American reactor pressure vessels.

The research is sponsored by the Nuclear Regulatory Commission.

What To Do With Weapons Plutonium

As nuclear warheads are dismantled in accordance with international agreements, large plutonium stockpiles are created. Also created is a problem: How can these bomb-grade nuclear materials be kept away from terrorists?

To consider ways to reduce the proliferation hazard of plutonium inventories in the United States and Russia, on December 4-5, 1995, ORNL served as the host site for a Joint U.S.–Russia Technical Summit Meeting on Plutonium Disposition. During the meeting, U.S. and Russian representatives exchanged important technical information concerning proposed options, such as encapsulating plutonium in glass, burying it in 4-kilometer-deep bore holes, or burning it in commercial power-producing nuclear reactors.

We're helping Russians evaluate use of reactors to reduce plutonium stockpiles.

ORNL was picked to host the first meeting of this type in the United States because of its U.S. leadership role for evaluation of reactor alternatives in the plutonium disposition program. ORNL researchers have examined the feasibility of extracting plutonium from dismantled weapons, converting it to a mixed oxide fuel (plutonium oxide mixed with depleted uranium fuel), and burning it in Canadian heavy-water reactors and U.S. light-water reactors. The Russians are studying the possibility of burning plutonium fuel in their light-water reactors.

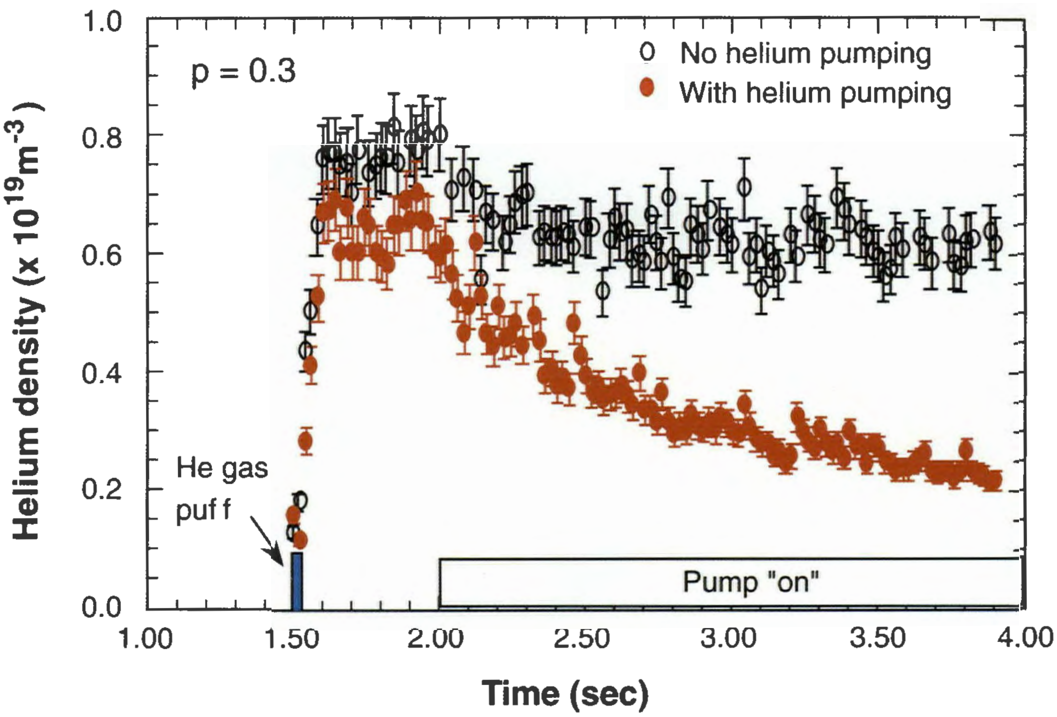
The meeting was completed successfully with the development of a detailed outline of the report to be produced by June 1996 to support the summit meeting between Presidents Clinton and Yeltsin. ORNL researcher Kent Williams was appointed U.S. co-chairman of a newly created Cross-cutting Cost Analysis Team, which will study the economics of the various plutonium disposition options. ORNL has been charged with working with the Russians to develop cost analysis methodology for Russian projects. This collaboration should create workable solutions that will safeguard the world's dangerous weapons materials and may extend its energy supplies.

This work was sponsored by DOE, Office of Fissile Materials Disposition.

Guiding Studies of Fusion Reactor Helium Exhaust

Our research on fusion's helium ash problem should aid design of an international fusion device.

Special people from around the world are needed to harness the energy source of the sun—nuclear fusion. International cooperation is the key to developing nuclear fusion reactors as a safe, abundant supply of energy. To design and build a fusion reactor that can produce electric power from fusion energy, nations are pooling their resources. Collaborative research in the international fusion community has led to the launching of the International Thermonuclear Experimental Reactor (ITER) Project, perhaps the largest international scientific venture ever undertaken.



ORNL studies at the DIII-D Tokamak in San Diego show that more of the energy-wasting helium "ash" formed as a by-product of fusion reactions is exhausted if divertor pumps are "on" (red) rather than "off" (black).

For the past decade, ORNL's fusion researchers have been intensely involved in multinational research efforts. In 1995, one of our contributions was recognized by ITER's Confinement and Transport Expert Group: Some of our researchers were invited to the group's meeting to report on the status of worldwide research on helium transport and exhaust in fusion reactors.

In nuclear fusion, two nuclei of heavy hydrogen (deuterium, which abounds in the ocean, and tritium) will fuse if held closely together and heated to a high enough temperature to overcome their natural repulsion. The products of this fusion reaction are neutrons, considerable energy, and helium "ash." If helium is not removed from the burning plasma, this impurity will gradually build up, quenching self-sustaining fusion reactions.

Our helium transport and exhaust group has been designing and performing experiments, collecting and analyzing data, and developing and validating research models. A goal of this work will be to develop a helium transport database that will guide design work on the ITER. It will provide information on results of experiments at small fusion devices, which can be extrapolated to the future ITER, a much larger reactor designed to show the technological feasibility of producing electricity from fusion energy.

It has been shown that magnetic fields can guide helium ions away from the plasma boundary into a diverter chamber from which the ions are exhausted. Based on data obtained from present-day experiments, researchers seek to optimize divertor configurations that more effectively remove helium. By solving the problem of helium exhaust, we will move closer to harnessing a special energy source that is virtually inexhaustible.

The research is sponsored by DOE, Office of Energy Research, Office of Fusion Energy Science.

We found a DNA marker for gender in hybrid willow trees, fast-growing sources of transportation fuel.

Nicholas McLetchie employs genetic engineering techniques like those used to determine the gender of a hybrid willow tree in an early stage of development.

Identifying Gender of Fast-growing Trees

Trees that grow up fast are in high demand. They can be used for fuel in transportation vehicles and for wood products. While they are growing, they can capture carbon dioxide from the atmosphere, helping to put the brakes on climate change.

Fast-growing trees are being cloned and nurtured for these purposes. One promising species is the hybrid willow tree. However, if the climate change predicted by some scientists ushers in higher temperatures and drought, hybrid willow trees of only one gender will be favored: male willow clones are generally more tolerant of dry conditions than are female willows.

It's not easy to tell a male willow from a female willow because trees of this species do not express gender until age 6 to 20 years. However, ORNL researchers in collaboration with Swedish scientists through the International Energy Agency have identified a potentially useful method for early identification of hybrid willow gender—a DNA marker.

The marker is present in all female hybrid willows and absent in all males. The marker will ultimately be used to isolate and characterize the DNA sequence responsible for gender selection. Use of this DNA sequence should greatly increase researchers' ability to identify highly productive, drought-resistant trees for biofuels. What was once a willow problem is no longer worth weeping over.

The research was supported by DOE, Office of Transportation Technologies, Biofuels Systems Division.

Superconducting Wire Developed

By learning how to lay a proper foundation, ORNL researchers have formed a promising new high-temperature superconducting wire. Combining a specially textured substrate, buffer layers that maintain the texture, and deposited films, the new wire can carry 710 times more current per unit area than conventional wire—without energy-wasting resistance. This development may pave the way for manufacturing practical, energy-saving wires for underground transmission cables, transformers, current limiters, large electric-power generators, and large motors used in paper and steel mills.

Twelve researchers from three ORNL divisions have produced a roll-textured, buffered metal, superconducting tape with a critical current density of 710,000 amperes per square centimeter in liquid nitrogen. The higher the current density, the greater the amount of electric current that can be transmitted through the wire. Standard household wires typically carry less than 1000 amperes per square centimeter.

High-temperature superconducting material chilled by liquid nitrogen (which costs 2% the price of liquid helium, the coolant for low-temperature superconductors) offers virtually no resistance to the flow of electric current. New electric devices wired with superconductors could take up less space, use less energy, and cost less. Although demand for electricity is expected to double by the year 2030, these devices could help reduce U.S. requirements for new power plants.

To make superconducting wire, the underlying substrate for deposited superconducting film must be flexible. It must be a perfect template with correctly oriented crystalline grains that align film grains to make a path for electric current. It must be reliably reproduced to form long lengths of wire.

At ORNL nickel-metal tapes are prepared using special rolling and heat treatment procedures. Thin buffer layers of palladium, cerium oxide, and yttria-stabilized zirconia are then placed on the nickel tapes by vapor deposition processes, such as electron-beam evaporation. The high-temperature superconductor yttrium-barium-copper oxide (YBCO) is then deposited on the conditioned surface by pulsed-laser deposition, a technique in which target materials in a vacuum chamber are vaporized by laser light so that they deposit on a template. Because nickel and YBCO are incompatible (nickel and copper atoms tend to trade places), the buffer provides a chemical barrier between the nickel and the superconductor while maintaining the texture.

One problem with high-temperature superconducting material has been that it tends to lose its superconductivity in an applied magnetic field. We have shown that the performance of our YBCO wire in a background magnetic field at liquid nitrogen temperature (77 K) is excellent, exceeding that of bismuth-based, powder-in-tube wires. This excellent performance is essential for applications in transformers, motors, and generators, where magnetic fields are present. In a 1-tesla field at 77 K, the critical current density of the YBCO wire is 150,000 amperes per square centimeter, and high critical currents are maintained in fields of up to 5 tesla. In addition, the critical current density at 64 K in a magnetic field of 1 tesla is as good as that of the metallic superconductors at 4.2 K, the boiling point of liquid helium.

High-current short wires 3 millimeters wide and 15 millimeters long have been produced using the ORNL process called rolling-assisted biaxial textured substrates, or RABiTS™. ORNL has applied for patents on RABiTS™ in the United States and certain foreign countries. A nonexclusive licensing agreement has been signed with Midwest Superconductivity of Lawrence, Kansas, for use of the technology in research and development. The agreement includes an option for rights to commercialize superconducting wire and tape. In a planned cooperative research and development agreement, Midwest has entered into a partnership with Westinghouse Science and Technology Center and Southwire Company for the development phase of the project with Oak Ridge.

Now that we have a super substrate, we may soon see practical use of superconductivity.

By developing a textured metal substrate, we've formed a new high-temperature superconducting wire that carries large amounts of current.

Fred List (left) and Patrick Martin observe sputtering of cerium oxide on textured nickel, the substrate for high-temperature wire capable of carrying large amounts of current. *Photograph by Tom Cerniglio.*

Funding for the project was provided jointly by DOE, Office of Energy Efficiency and Renewable Energy, Office of Utility Technologies and by DOE, Office of Energy Research, Division of Materials Sciences.

Reducing Costs of DC Power Transmission

One way to be sure to get power to the people when electricity is in high demand is to connect utility networks. An electrical utility in need can then draw power from another utility's network or even from small private generators of electricity. Transmitting high-voltage, direct-current (HVDC) power between networks requires back-to-back converter systems to overcome tiny inherent differences in generating frequency and phase between networks.

Back-to-back converters, which change alternating current (ac) to direct current (dc) and back again, are expensive components in HVDC transmission stations and switchyards. To reduce the cost of HVDC converter stations, researchers at ORNL have completed developing and testing the world's first multilevel back-to-back converter system for HVDC transmission.

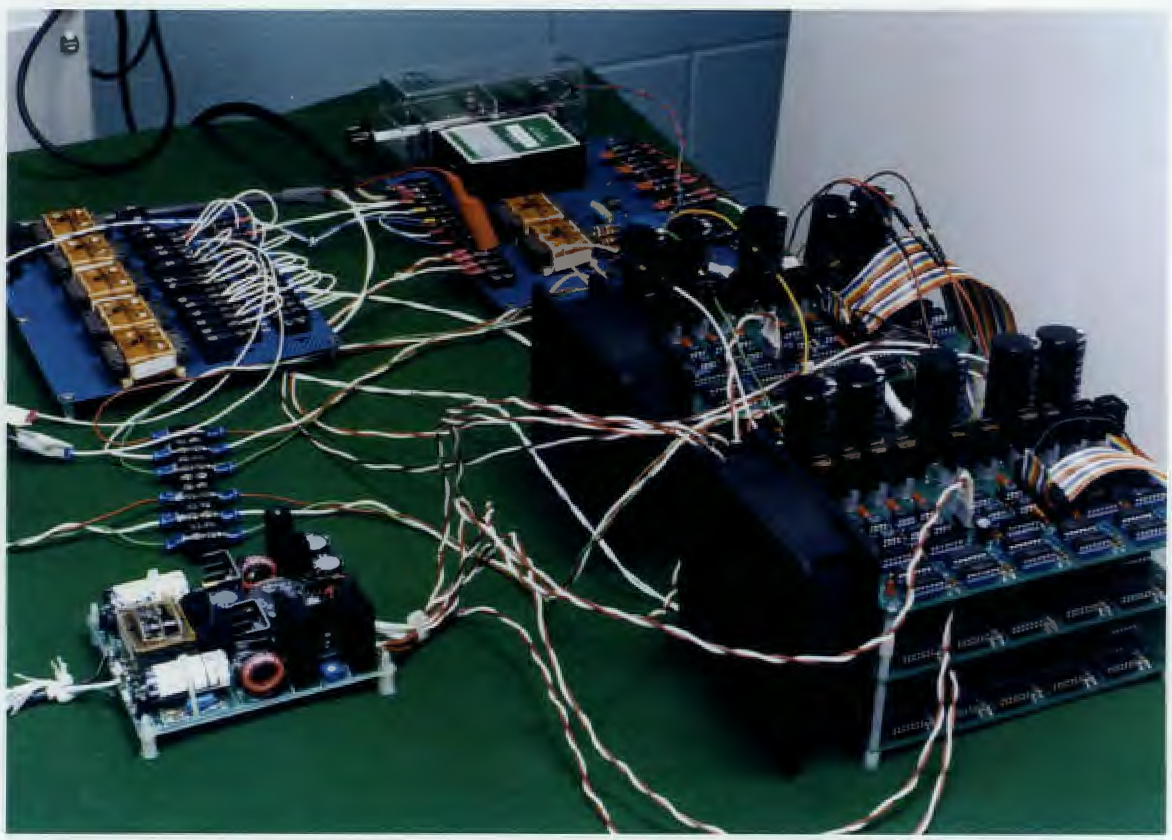
The multilevel converter synthesizes sinusoidal voltage—sine waves that resemble staircase steps on a computer screen—using multiple levels of voltage from different capacitors. The invention eliminates three out of four major HVDC converter station components found in traditional transformer-coupled stations. No longer needed are bulky and expensive transformers, large ac and dc filters, and switch-operated capacitors that correct power factors (the ratio of power to the product of voltage and current). As a result, engineering and installation costs are significantly reduced.

The converter developed at ORNL offers nearly distortion-free output voltage. It may also be used in other high-voltage applications such as unified power flow controllers (which enable power systems to be operated closer to peak capacity), industrial motor drives, electric traction drives for high-speed rail transportation (including that propelled by power-hungry magnetic levitation), and reactive power compensators that stabilize power system voltage.

Deployment of multilevel converter-based systems at HVDC stations throughout the nation will enable the use of two instead of three transmission cables for ac systems, reducing power transmission and distribution costs and real estate costs by at least 33%. In some designs, the earth is used as the return current path, so the savings can be as high as 66%. In addition, dc transmission does not produce electromagnetic fields, which have been a major health concern of the public. It's good to get power to the people, and it's even better to minimize the impact on their pocketbooks.

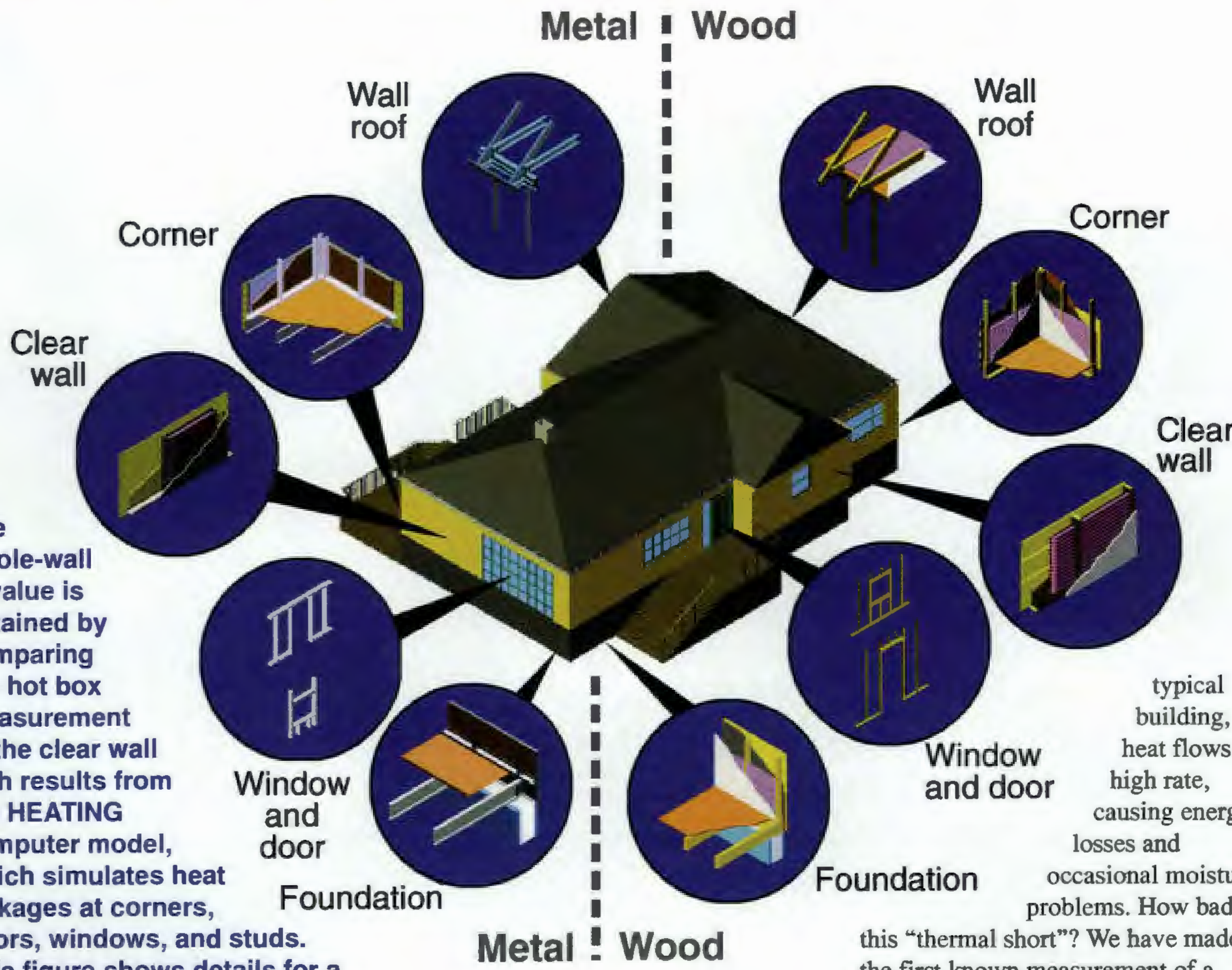
Funding for this development was provided by DOE Office of Energy Management to the Power Systems Technology Program in the Energy Division.

We've developed a back-to-back converter that could cut costs of high-voltage DC power transmission.



View of the back-to-back converter developed at ORNL to change alternating current to direct current and back again.

We've created a procedure to help users measure R-value in walls and a computer model that predicts energy losses from wall-floor connections.



The whole-wall R-value is obtained by comparing the hot box measurement of the clear wall with results from the HEATING computer model, which simulates heat leakages at corners, doors, windows, and studs. This figure shows details for a standard 2 × 4 inch wood frame wall and a metal frame wall, which is gaining popularity in residential construction.

New Wall Ratings and Thermal Shorts

What's the R-value in your walls? The answer used to be the R-value of your wall insulation in wood-frame walls. But now R-value, or resistance to heat flow, can be measured in the whole wall, not just the insulation, using ORNL's new wall testing and rating procedure. We are performing whole-wall testing and rating for users at the Buildings Technology Center, a DOE user facility at ORNL. We have already worked with 7 firms and are currently working with another 4; about 36 firms expressed some interest. Users pay $3000 to $15,000 each for testing in our new Rotatable Guarded Hot Box and for computer modeling. Total wall R-value ratings allow comparisons of thermal resistances of dissimilar walls. This capability is important because of the growing use of alternative wall systems and construction materials such as metal. We have put the performance information in a database (http:www.cad.ornl.gov/kch/demo.html) so home designers, builders, realtors, and buyers can predict ratings for new wall systems and materials. Several state energy agencies are considering adopting our procedure.

* * *

At the junction of a conventional concrete floor and masonry wall in a typical building, heat flows at a high rate, causing energy losses and occasional moisture problems. How bad is this "thermal short"? We have made the first known measurement of a thermal short in the Rotatable Guarded Hot Box. The energy losses and potential for excessive moisture condensation are worse than were expected. Based on the heat-loss measurements, a recommended simplified computer model that predicts energy losses from wall-floor connections has been developed and was presented to the American Society of Heating, Refrigeration, and Air-Conditioning Engineers in June 1995. The work is part of a cooperative research and development agreement with Enermodal. The information could lead to improvements in construction of floors and walls to make better connections and help seal the building envelope.

Funding for the research is provided by DOE, Office of Building Technologies. ornl

Instrumentation, Manufacturing, and Control Technologies

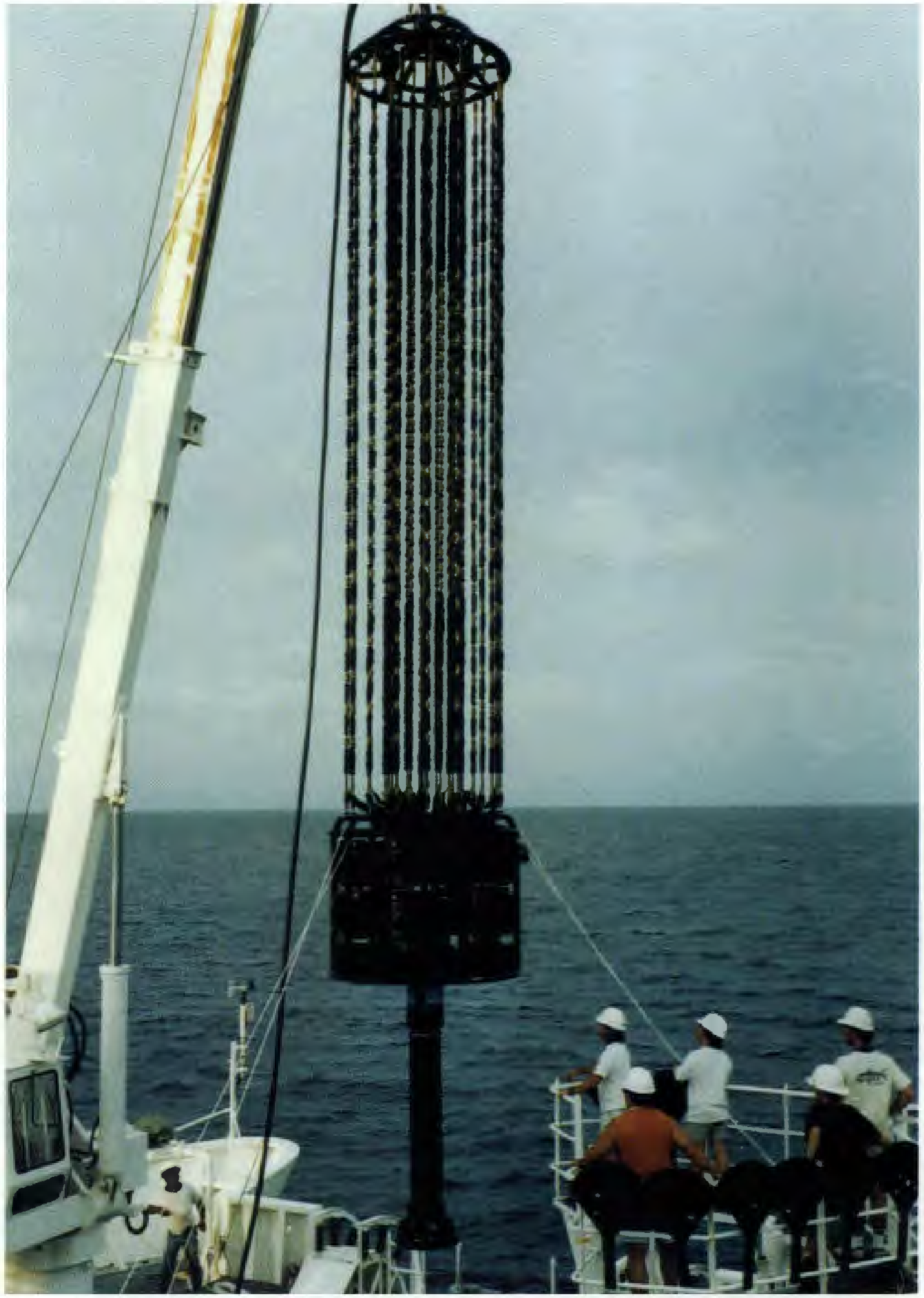
We have devised instruments to measure or monitor radiation levels, electromagnetic fields, temperatures, sounds, and the weight of gases. We have conducted testing to hasten the commercialization of new manufacturing technologies. We have created methods to control a variety of systems. The capabilities represented by this core competency span the range from basic research in materials and processes through prototype development to production-scale facilities for precision manufacturing and inspection at the Oak Ridge Centers for Manufacturing Technology.

Because of our skills in measurement science, we have developed miniature, automated sensors that measure barely detectable quantities. By integrating these sensors with electronics and computing capabilities, we have developed early warning systems and advanced control technologies. Thanks to our instrumentation and control expertise, we received two R&D 100 awards in 1995 in this area—one for a gravimetric gas flow calibrator (that calibrates gas flow meters) and the other for a magnetic spectral receiver (that monitors magnetic fields that may degrade the performance of power plant control instruments).

Oak Ridge's strength in manufacturing technologies reflects a unique three-site collaboration involving ORNL and the Oak Ridge Y-12 Plant and K-25 Site. Within this partnership, ORNL's research and development capabilities in materials and processes are meshed with the precision manufacturing, fabrication, and inspection skills of Y-12 Plant personnel and with state-of-the-art pollution prevention technologies at the K-25 Site.

We've developed a system that measures "whispers" from U.S. submarines in the "noisy" ocean.

ORNL Measures the Undetectable: Submarine Noise



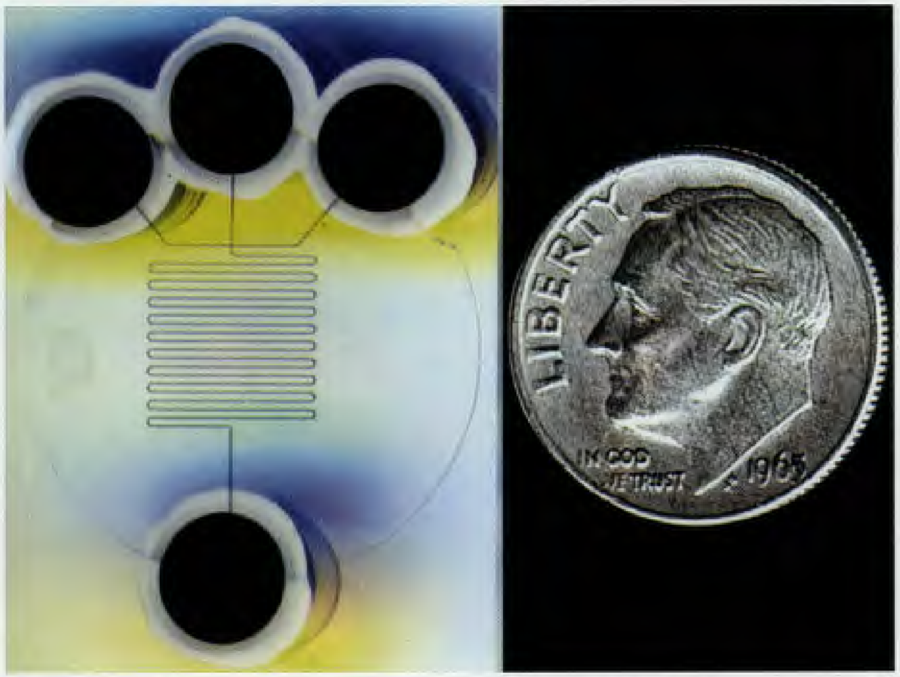
U.S. Navy personnel prepare to deploy one of the advanced ORNL-developed acoustic monitoring systems off the bow of the *USNS Hayes.* The latticework of hydrophones is strung above pressure vessels containing instruments.

To better escape detection as they ply the seas, American submarines are becoming quieter. So, before sending its new subs out to sea, how does the U.S. Navy know if its latest immersed stealth technology is as quiet as it's designed to be and otherwise operates as specified? The Navy has obtained its answers from the world's most advanced underwater acoustic measurement system, developed by ORNL. This system, which detects the equivalent of whispers in a noisy crowd, precisely measures acoustic images, or signatures, of noise radiated from U.S. submarines. It provides acoustic measurements of energies that are normally undetectable because their level is below the ocean's background noise.

By combining our expertise in computing, instrumentation, and system integration, we have designed and built electronic devices and developed signal processing technologies that provide accurate measurement of sounds so small they would otherwise be undetectable. We have met Navy requirements to qualify the operating characteristics and specifications of the newest U.S. submarines—the *SSN 21 Seawolf* and the next-generation submarines planned for production in the next 10 years. Our system ensures that acoustic emissions from these vessels are kept at levels below their design limits. The Navy's ability to maintain stealth in the U.S. submarine fleet depends largely on ORNL's ability to measure the sound of silence.

Funding for ORNL's development work in the Acoustic Measurement Facilities Improvement Program was provided by the U.S. Navy, Naval Surface Warfare Center, Carderock Division.

ORNL's MicroBioLab chip could be used for gene screening, DNA fingerprinting, and drug research.



This "lab on a chip" has been used to analyze DNA.

Mike Ramsey shows the MicroBioLab chip developed at ORNL. *Photograph by John Smith.*

Lab on a Chip Analyzes DNA in a Droplet

We know one way to shrink a chemistry laboratory: build a "lab on a chip." We have developed a postage stamp-size MicroBioLab chip that can dissect DNA in a droplet. Compared with today's commercial analytical instruments, it works 10 times faster, analyzing DNA in only 5 minutes instead of an hour. Also, it can chemically analyze a liquid sample 10,000 times smaller, saving materials. In addition, less labor is required because it's computer controlled.

Such a cost-effective, time-saving chip could be built for genetic diagnosis, DNA fingerprinting, and drug research. It could screen for people carrying genes that predispose them to developing breast cancer, becoming obese, or having children with cystic fibrosis. To make such an analysis, it is hoped that only a few blood or skin cells in a drop would be required.

The technology could also have forensic uses such as DNA fingerprinting—a technique for comparing molecular characteristics of blood at the crime scene with those of blood from victims and suspects. One person could collect blood samples at the scene of the crime and do an analysis then, reducing the chance of contamination by other people's blood.

Another possible use is in drug research. Because enzyme-inhibiting chemicals are expensive and hard to come by, drug companies are interested in technologies for analyzing very small samples to find potentially effective drugs.

Thin as a microscope slide, our glass microchip has been etched to form interconnected chambers and channels, just beneath the surface. Charged molecules in a tiny liquid sample are mixed in a chamber and "pumped" through hairlike channels by an applied electrical field. The molecules glide around the hairpin turns of a winding capillary channel, covering an area the size of the face of a wrist watch.

Our microminiature sensors can detect and measure heat, sound, water, and gases.

Taking a break from his work with an atomic-force microscope, Thomas Thundat observes the magnification of a straight pin, an insect, and an ORNL-developed cantilever sensor, like the one he's holding. By comparison, the cantilever sensor is the smallest of all. These microscopic sensors can be used to measure heat, sound, water and gas concentrations, and radiation.

Before DNA molecules—cut into fragments by enzymes—enter a separation channel where they are separated by size and electric charge, they react with a fluorescent dye. The dye causes the fragments to give off light when a laser beam is shone on them just below the separation channel; the larger the separated fragment, the stronger the fluorescence. The detected light intensities are fed to a computer, which sorts through signals from separated fragments to provide a sample analysis. MicroBioLab chips may be small, but the potential is large.

The research was supported by DOE through ORNL's Laboratory Directed Research and Development Fund.

Microcantilevers: Sensors with Sensitivity

Thanks to a problem with a high-tech microscope, ORNL researchers have developed microscopic sensors—hairlike, silicon-based devices that are at least 1000 times more sensitive and 1000 times smaller than currently used sensors. They can detect and measure relative humidity, temperature, pressure, flow, viscosity, sound, natural gas, mercury vapor, and ultraviolet and infrared radiation. They also show potential as biosensors—devices that can detect DNA sequences and proteins.

In 1991 an ORNL researcher was using an atomic-force microscope to examine the effect of humidity on DNA. The humidity affected the performance of the microscope's cantilever, which is used to map the atomic mountains and valleys of surfaces, just as a phonograph stylus traces record grooves. It occurred to the researcher that the cantilever is a potential sensor. Fortunately, newly available micromachining techniques make it possible to fabricate microcantilever sensors that are rugged and extremely sensitive yet cost little and consume little power.

Microcantilevers of silicon or silicon nitride have been made that are smaller than the period at the end of this sentence. These "microscopic diving boards" project from miniature chips about the size of a grain of rice.

ORNL researchers have shown that a microcantilever would bend in a measurable way if its tip is coated with a material that attracts another material from the air. For example, a gold-coated cantilever absorbs mercury vapor, which stiffens the cantilever, causing it to bend and changing the way it vibrates. A gelatin tip absorbs water, measuring humidity. A silicon microcantilever coated with aluminum bends more with rising temperature because aluminum expands more than silicon. Such a device can measure temperature and even detect infrared radiation and

A neutron analysis system can disclose contents of coal and cement and detect drugs and explosives.

ORNL's nonintrusive inspection technique that uses neutrons can detect cocaine in pallets of sugar.

heat-generating chemical reactions. When set in motion, microcantilevers have a natural vibration that changes in the presence of sound waves or a fluid (enabling measurements of viscosity and pressure).

Changes in cantilever position or vibration rate can be detected by measuring wobble in reflected laser beams. Future silicon devices, however, will probably be based on piezoresistance—changes in electrical resistance induced by increased bending or reduced vibration. One of our patented technologies has been licensed to Consultec, Inc., which has fabricated a prototype mercury vapor sensor and an infrared thermometer. Thanks to a problem, ORNL devised a new class of sensors that may help industry find economical solutions.

DOE's Office of Health and Environmental Research funded this work.

Neutron Technique May Help Coal, Cement Industries

A nonintrusive inspection technique that probes samples with neutrons can analyze the content of coal and cement and detect explosives and drugs. It also shows promise for locating plastic and wooden land mines.

Developed by ORNL and Western Kentucky University (WKU) researchers, the pulsed fast-thermal neutron analysis system bombards a sample with pulses of fast and slow, or thermal, neutrons. Fast neutrons collide with some atomic nuclei, triggering the release of gamma rays. Between pulses, thermal neutrons are captured by other nuclei, resulting in emission of gamma rays. Detectors measure energies of the combined gamma rays, which are unique for each element.

Gamma-ray fingerprints permit accurate determinations of concentrations of hydrogen, carbon, oxygen, nitrogen, chlorine, sulfur, and other elements in samples. Using both fast and slow neutrons allows detection of more common elements. For example, carbon can be readily identified using fast, but not slow, neutrons; the reverse is true for chlorine. The new technique's power lies in its ability to measure elemental content on-line during industrial operations.

Negotiations are under way to install a prototype pulsed-neutron generator system at an operating coal-fired power plant. The coal industry has a strong need for this on-line analytical capability. To price coal accurately or blend it to make it cleaner, it helps to know its sulfur content. To operate a coal power plant as efficiently as possible, it is important to know how much carbon and oxygen are in the coal. To cut back deposits that clog pipes in boilers, it is wise to burn coal low in chlorine. Because chlorine is a "poison" in crystallization of cement, manufacturers of cement have expressed a desire for an on-line analytical capability for quality and process control.

The neutron generation system shows promise for other applications. WKU researchers have demonstrated the technique's ability to distinguish between actual and mock explosives in munitions shells in military proving grounds to speed up environmental restoration and to inspect pallets of rice, sugar, or coffee for cocaine. ORNL researchers are investigating whether the technique can guide the safe removal of land mines.

The research has been sponsored by DOE's Experimental Program to Stimulate Cooperative Research.

Electron Beams May Cure Plastics Problem

To cut manufacturing costs, we're adapting and commercializing electron-beam curing for forming high-strength plastics for transportation vehicles.

Lightweight, fiber-reinforced plastics that perform under harsh conditions are being used in boats, jet aircraft, and spacecraft. These high-performance polymer matrix composites (PMCs) are found in wings, stabilizers, engine housings, tail assemblies, fuselage sections, and aerospace structures. Because they are both light and strong, PMCs may also be the lightweight structural material chosen to replace steel for the future Supercar—a vehicle being developed under the Partnership for a New Generation of Vehicles that will offer high efficiency and low emissions at an affordable price.

The problem with PMCs lies in the high cost to manufacture them. Currently, the high-strength plastic is formed from fibers held together by polymers, compounds of high molecular weight that have millions of repeated linked units—each a relatively simple and light molecule. To cure the composite, chains of polymers mixed with fibers must be linked by creating covalent chemical bonds in which electrons are shared. This cross-linking is achieved today by thermal curing using gas-fired ovens or steam-operated autoclaves. Thermal curing uses considerable energy to heat and cool the material, is time consuming, and can induce residual stresses in the finished part. It also requires use of a hardener, which can be a source of potentially toxic emissions.

An alternative curing process that uses less energy, requires minutes rather than hours, emits no pollutants, and is potentially less costly is now being investigated in Oak Ridge. ORNL researchers are leading a national effort to advance and commercialize a PMC curing technology that would use nonthermal electron beams from a high-energy accelerator. This technology is now used for coatings and sterilization of foods and medical supplies.

ORNL conducts experiments in producing polymer-composite parts using a continuously operated electron-beam system in western Canada. The electron beam scan horn at top center directs and controls distribution of electrons to composite test parts.

Participants include researchers at the Oak Ridge Centers for Manufacturing Technology, DOE's Sandia National Laboratories, and 10 industrial partners involved in a cooperative research and development agreement (CRADA) supported by DOE.

The goal is to develop electron-beam technology that can produce better products in higher volumes than are generated by thermal curing and at lower costs. By comparison, electron-beam curing has the potential to reduce tooling and manufacturing costs and curing times; simplify processing; improve part quality; and make unique products not producible in any other way. The process is also environmentally friendly: hardeners are not required in the resin, and no volatile substances in the resin escape to the atmosphere because of the low cure temperatures and the material's composition.

ORNL researchers played an important role in developing new chemistry to inexpensively modify the PMC base-resin material, rendering it curable by electron beams. They identified a group of photoinitiators that enables the material to be cured under a range of temperature conditions. The photoinitiators allow electron beams to ionize the polymer chains so cross-linking occurs. The patented process has been licensed to two manufacturers of resin systems.

Results of the CRADA so far indicate the concept is technically and economically viable. Four independent economic studies confirm a 50% reduction in manufacturing cost. Continued success with this project should provide the plastics industry with the stimulus to produce affordable composites for a broad range of uses by the transportation industry.

We've developed a way to measure and control radio frequency power levels for making computer chips.

ORNL's Tony Moore (in white shirt) points out features of the rf matcher invented at the Laboratory. The small device at the back of the table is an ORNL-developed sensor for the rf system for accurately measuring and controlling rf power levels in plasma processing equipment used to produce semiconductor chips. *Photograph by Steve Eberhardt.*

RF System May Improve Chip Production

As prices of computer chips fall and costs of chip processing equipment rise, the U.S. semiconductor industry seeks to become more competitive. Its goals are to pack more circuits onto semiconductor wafers and produce more high-quality wafers per day. One approach to achieving these goals is to get better control over plasma etching of wafers. In this process, hot ionized molecules, such as a gaseous compound of fluorine, etch integrated circuit patterns many times smaller than a human hair.

Sometimes the plasma is not well controlled because of fluctuations in radiofrequency (rf) power levels that result in variations from wafer to wafer. If these variations are large enough, wafers can be defective.

One of the keys to producing a uniform etch is accurately controlling the rf power that generates the plasma. The rf energy is used to break down the gas and ionize the etch gaseous compound. Then neutral atoms fall out of the plasma onto the wafer, etching the surface chemically.

Under a CRADA between DOE and SEMATECH, ORNL researchers have developed a technique for accurately measuring and controlling rf power levels in plasma-processing equipment. The rf system controls delivered power to plasmas at least 10 times faster and more accurately than systems routinely used throughout the industry. This novel system offers the potential for improved yield and increased throughput of high-quality wafers from plasma etch equipment.

The measurement technique uses two highly nonobtrusive sensors (invented by ORNL researchers) that determine whether the impedance (resistance and capacitive reactance) in the plasma and the rf generator match. The sensors take data on impedance mismatches in equipment and cables that carry the rf power and feed it to a microprocessor that controls a novel electronic rf power matching network that has no moving parts (invented by ORNL).

In a few milliseconds, the controller tunes the rf matcher so that rf impedance matches the changing electrical impedance of the plasma in the etch equipment. The controller also rapidly adjusts the rf power level of the generator to compensate for power losses along the delivery path to maintain constant delivered power to the plasma. The combination of accurate sensing and rapid controlling of rf power offers better plasma control, fewer wafer-to-wafer variations, and increased production throughputs with higher yields.

Through better control of plasma etching, the U.S. semiconductor industry can improve its competitiveness in the world market.

Optics Testing Technology Now Affordable

An affordable optics measurement system has been developed through an ORNL CRADA with a small business.

The optics industry is focused on finding cost-effective technologies for producing better, smaller, and lighter optical devices. The industry also seeks to avoid the types of errors that gave the Hubble Space Telescope blurry vision and to embrace the technology that ensured its correction.

Although mirrors and lenses with spherical surfaces are relatively easy to manufacture and test, optics manufacturers are increasing production of optical components that have not quite spherical, or aspheric, surfaces (as in the space telescope's parabolic mirror). Although aspheres have been produced for centuries, technology for manufacturing them has significantly improved only in recent years. Use of aspheric components significantly reduces the number of optical elements required, making possible lighter, smaller optical packages.

Curt Maxey aligns the CGH Null Adapter using a specialized computer-generated hologram. In conjunction with custom CGH null lenses, the product enables aspheric optics to be tested with conventional interferometers to ensure they have the right shape. *Photograph by Lynn Freeny.*

Traditionally, optics manufacturers machine-ground telescope mirrors to about the right shape. To get a smooth enough curved surface to capture and focus light, opticians would hand-polish the mirror. Nowadays, an increasing number of optical components are formed and polished by computer-controlled processes. Single-point diamond turning is now routinely used to rapidly produce precision aspheric optics in metals, plastics, and selected crystalline materials. Unfortunately, testing technology has lagged behind precision manufacturing, contributing to the high cost.

To determine if an aspheric lens or mirror has the right shape, an optical measuring system is used. Light from a laser is bounced off the optic and back through an interferometer, forming an interference pattern. Conventional null lenses bend the light from the interferometer into a shape that matches the aspheric optic. These patterns are imaged and analyzed to determine if and where the optic requires more polishing. Because the accuracy of a conventional null lens depends on alignment of individual lens elements, it can give erroneous results if assembled with an error in spacing. Such a null lens deficiency resulted in the wrongly shaped mirror in the Hubble Space Telescope.

Much of the uncertainty in testing aspheric optics has been removed by the development of computer-generated holograms (CGH). Using diffraction, the phenomenon that produces the rainbow of colors in a compact disc, a CGH null lens bends light to match the shape of an aspheric optic. CGH technology is now considered the most reliable in the world for testing aspheric optics. CGH lenses were used to certify the accuracy of aspheric optics that were later installed during a space mission to correct the vision of the Hubble Space Telescope.

Because of the complexity of CGH technology, only a few specialized optical manufacturers could afford it. Now, thanks to a CRADA between ORNL and Diffraction International of Minnesota, reliable CGH technology is now affordable and available for all optics manufacturers. Diffraction International's revolutionary product, the CGH Null Adapter, is a simple accessory that allows accurate testing of aspheric optical surfaces using standard commercially available test equipment. Significantly, the product cuts the cost of the technology about 90%, from more than $100,000 to $10,000.

To hasten the commercialization of the CGH Null Adapter, ORNL metrologists tested early prototypes and provided detailed feedback to Diffraction International on the product's performance. Through a series of tests with different aspheric optics and measurement systems, the CGH Null Adapter evolved to its current form. Now, it's catching the eye of the cost-conscious optics industry.

The CRADA was funded by the DOE Energy Research Laboratory Technology Applications Program.

ORNL Boosts Police Security for Olympics

Our command, control, and scheduling system helped the Atlanta police keep order during the Summer Olympics.

Bob Hunter checks the computer display showing the buildings (pink blocks) and streets (red lines) of Atlanta and Olympic Games venues (yellow and green spots). ORNL's computer system helped coordinate the relocation of police officers in response to emergencies. *Photograph by Tom Cerniglio.*

"Security for the Atlanta Olympics should be the best in modern history, thanks in part to the fusion of computer, communications, and police sciences at a level never before attempted." So said General Barry McCaffrey, director of the White House Office of National Drug Control Policy. The advanced technology package, called the Police Command and Control System, was developed for his Counterdrug Technology Assessment Center by ORNL. It was part of the Clinton administration's plan to fight drugs and crime in the Atlanta area during the 1996 Summer Olympic Games.

This command, control, and scheduling system provided information vital to the creation of future systems for use by local, state, and federal law enforcement agencies. During the Olympics, the system gave the Atlanta Police Department a critical response advantage as it exercised responsibility for security during the games.

The Atlanta Police Department, which worked directly with ORNL to develop the computer system, gave the system good reviews. The pioneering Police Command and Control System, says the department's Major Jon Gordon, "gives real-time knowledge of and maximum access to every security resource available to meet a wide variety of potential problems, challenges, and instant crises. During the Olympics, these ranged from vehicular traffic gridlock miles from the events to possible criminal activity at one or more of the games' venues."

The ORNL team specializes in redefining problems normally solved on expensive workstations so they can be handled by low-cost, easy-to-use PCs. Use of PCs significantly reduced training and maintenance requirements for the Atlanta Police.

The chief of police used the system's "central manager" computer to analyze ongoing situations during the Olympics to assist in making critical decisions on police deployment. For example, when a pipe bomb went off in Centennial Olympic Park, the system provided an immediate assessment of the situation. As a result, the police chief could close the minimum number of streets to cordon off the area and direct police personnel to the scene to provide public safety support. Should a situation have required moving police forces to address security problems at a new location, the central manager could have automatically scheduled the relocation of nearly 2000 police and minimized the impact on other venues.

Most of the data (e.g, breakdown of a squad car, excessive traffic congestion, people injured in an accident) were communicated to the central manager system from police using other computers in the Olympic ring—the "field manager systems." The command-and-control system can also be used for complex analysis of patterns of crime from tens of thousands of pieces of information.

This project was supported by the White House Office of National Drug Control Policy. ornl

Advanced Materials Processing, Synthesis, and Characterization

Materials—the right stuff—form the key to progress in energy efficiency; environmental protection and remediation; and energy production through fossil, nuclear, and alternative technologies. ORNL's program in materials research and development (R&D) is one of the nation's largest, as well as one of the most respected internationally. Our programs cover the full spectrum from materials synthesis, processing, and characterization through modeling and performance evaluation. A key factor in the success of these programs is the integration of basic, applied, and industrial R&D.

This multidisciplinary research focuses on several important classes of materials, including ceramics and composites, metals and alloys, superconductors, and thin films. In addition to providing scientific leadership, ORNL's materials programs are major contributors to technology.

In 1995 ORNL received 5 R&D 100 awards, 3 of which were for advances in the materials sciences. Our prize-winning developments were the Exo-Melt™ process, which provides a furnace-loading method for low-cost, energy-saving production of nickel and iron aluminides, which have industrial uses; gelcasting, a new ceramic-forming process for making high-quality, complex-shaped ceramic parts that is being advanced to the commercialization stage by AlliedSignal and other companies; and (in collaboration with 3M researchers) the 3M ceramic composite filter, a fiber-reinforced ceramic composite candle filter that removes particulates from hot gas streams in pressurized fluidized bed combustion systems and coal gasification plants, protecting turbine blades needed for electricity generation.

Past products that evolved from our integrated programs have an estimated private-sector value of more than $300 million a year. Commercial applications of ORNL technologies include artificial hip joints, furnace fixtures for manufacturing structural steel and automobile parts, dies for making aluminum cans, filters to reduce emissions from coal-burning plants, new pressure vessel steels for power plants, and ceramic drills and cutting tools.

ORNL's materials program embraces an unparalleled infrastructure of specialized equipment, facilities, and expertise. These are central to extensive interactions and collaborations with both the private and public sectors. The High Temperature Materials Laboratory (HTML) and the Shared Research Equipment Program offer state-of-the-art instruments for characterizing microstructure and properties of materials with the aim of linking one to the other. The High Flux Isotope Reactor houses the Neutron Scattering Research Facility for characterizing the structure of materials with neutron probes. The Surface Modification and Characterization Research Center includes unique facilities for ion implantation of materials to improve their properties. And the Residual Stres User Center combines strengths of HTML and the Neutron Scattering Research Facility to measure residual stresses in welds, automobile brake rotors, and other materials and machines.

Reaction Synthesis: Take a Powder, Make a Product

At high temperatures, nickel and iron aluminides modified at ORNL are stronger than stainless steel, exhibit ductility, and resist corrosion. But as blocks, sheets, or tubes, these heat-resistant alloys also resist being shaped into a final product because they're so brittle at room temperature. We have found a promising solution: form the alloy from metallic powders using internal heat generated during the powders' reactions. This "reaction synthesis" method is considered attractive for producing aluminide products in desired shapes, with little or no machining.

Reaction synthesis may also be used to produce highly dense aluminide products for structural uses. Aluminides have many uses now, but because they are porous, they are too weak to bear heavy weights. Using reaction synthesis we have reduced the porosity from 3% to 0.1% in a ductile nickel-aluminide product.

ORNL researchers developed the Exo-Melt furnace concept for efficiently and safely melting and casting alloys of nickel and iron aluminide. *Photograph by J.W. Nave. Computer photo enhanced by Mark Robbins.*

Reaction synthesis could lower costs in two ways. Aluminide products can be formed directly from elemental powders rather than in two steps (melting and casting), and the self-generation of heat during alloy formation reduces energy requirements.

In reaction synthesis of aluminides, powders of aluminum and the other metal are mixed. The unreacted samples are shaped into disks of a desired shape and heated in a chamber under vacuum to a temperature that initiates a self-sustaining, heat-liberating reaction, like burning logs in the fireplace. By applying a little pressure, we found we could squeeze out the material's pores, making it almost fully dense.

Using high-speed videotaping equipment, we studied the reaction behavior of iron aluminides during synthesis in air. We found that the reaction rate depends on compact composition and powder particle size; it increases with greater aluminum content, and it drops with increasing powder size.

Another ORNL group has shown that reaction synthesis, not under vacuum or pressure, can be used to melt and cast ingots. This group developed the Exo-Melt process by extending principles of reaction synthesis to the melting and casting of iron aluminide (Fe_3Al) and nickel aluminide (Ni_3Al). This process, which uses half as much energy as traditional processes and addresses safety concerns of the alloy preparation industry, received an R&D 100 Award in 1995.

The key to the success of the Exo-Melt process is the furnace-loading sequence. As the aluminum melts and comes in contact with the heated nickel at the top of the furnace, NiAl forms, releasing large amounts of heat. On its way down, the superheated NiAl liquid dissolves alloying elements (boron, chromium, molybdenum, and zirconium), found by ORNL to make the alloy ductile and strong at high temperatures. Additional NiAl reacts with the nickel at the bottom of the furnace to form the desired alloy—Ni_3Al.

Using the Exo-Melt process, four vendors now melt and cast highly durable products from nickel aluminides for the steel, automobile, and tool industries. Products include transfer rollers for heat-treating steel plates in steel mills and "furnace furniture"—assemblies that hold automobile parts during high-temperature treatment to harden their surfaces.

As a result of these successes, a unique facility has been developed at ORNL to study reaction synthesis of intermetallic alloys. The facility will be used to study processing parameters and the feasibility of forming near-net-shape products. Someday industry may find this emerging method of making products from powders too good to resist.

This continuing intermetallics success story and example of the integration of research and technology developments highlights the value of cooperation among several programs in DOE's Office of Energy Research that are supporting this work. They are Basic Energy Sciences, Energy Efficiency, Fossil Energy, and Energy Research Laboratory Technology Applications programs.

ORNL-3M ceramic composite filters for future coal power plants are a technology transfer success.

David Stinton (left) and Rod Judkins have worked on developing and commercializing the 3M hot-gas ceramic filter (shown here), which has been tested in the Westinghouse Advanced Particle Filter System at the Tidd Pressurized Fluidized-Bed Combustion Demonstration Project in Brilliant, Ohio (interior shown at right).

Filters for Clean Power Plants

The most efficient power plants of the near future are likely to use hot gases from coal to drive a gas turbine and produce steam that will spin a steam turbine. A technical problem, however, has marred the performance of pilot plants of these pressurized fluidized-bed combustion (PFBC) and integrated coal gasification combined cycles. Candle filters used to remove hot-gas particulates that erode and corrode gas turbine blades survived only a short time. ORNL researchers recognized the need for a longer-lasting filter, so they developed a gas particulate filter made of a novel ceramic composite. Their invention was then licensed to the 3M Company.

ORNL and 3M researchers collaborated on improving the filter to make it a commercial product. To see if it could endure real-world conditions, Westinghouse Electric Company tested the filters in a combined-cycle demonstration plant. In December 1994, ten full-size, 3M candle filters were installed in a filter vessel at the Tidd PFBC demonstration project, which was funded by the DOE Clean Coal Technology Program, at Ohio Power Company's power plant in Brilliant, Ohio. The system was operated until about March 31, 1995.

On April 26, 1995, a borescope examination of the interior of the filter vessel was performed. All ten of the filters were in place and appeared to have functioned well. The filters were removed during the next few weeks for nondestructive and destructive examination. All of the filters had performed well, and all had retained properties that suggested they could perform for times acceptable for commercial operation of a PFBC plant. Additional filters are in a second PFBC demonstration project in Karhula, Finland. The filters' versatility has been shown by their excellent performance in a coal gasification plant in Germany. As a result of the successful demonstrations, 3M has increased its production capability for the filters. ORNL's small candle filter effort has sparked the development of a business worth millions of dollars.

The research and technology transfer efforts were supported by DOE Office of Fossil Energy's Advanced Research and Technology Development Materials Program and the Morgantown Energy Technology Center.

Making Nanocrystals with Ion Beams

As their semiconductor "brains" get smaller, computers get smarter and faster. In the past few decades, researchers have shrunk many materials devices to increase computer performance. When sizes are decreased to billionths of a meter (nanometers), materials are reduced to small clusters of only hundreds of atoms. Such nanoclusters, or nanocrystals, often exhibit fascinating physical properties very different from those of the bulk material. For example, electronic energy levels and optical properties such as absorption and emission of light can be shifted dramatically when dimensions of crystallites approach dimensions of fundamental excitons (electrically neutral excited states of insulators and semiconductors).

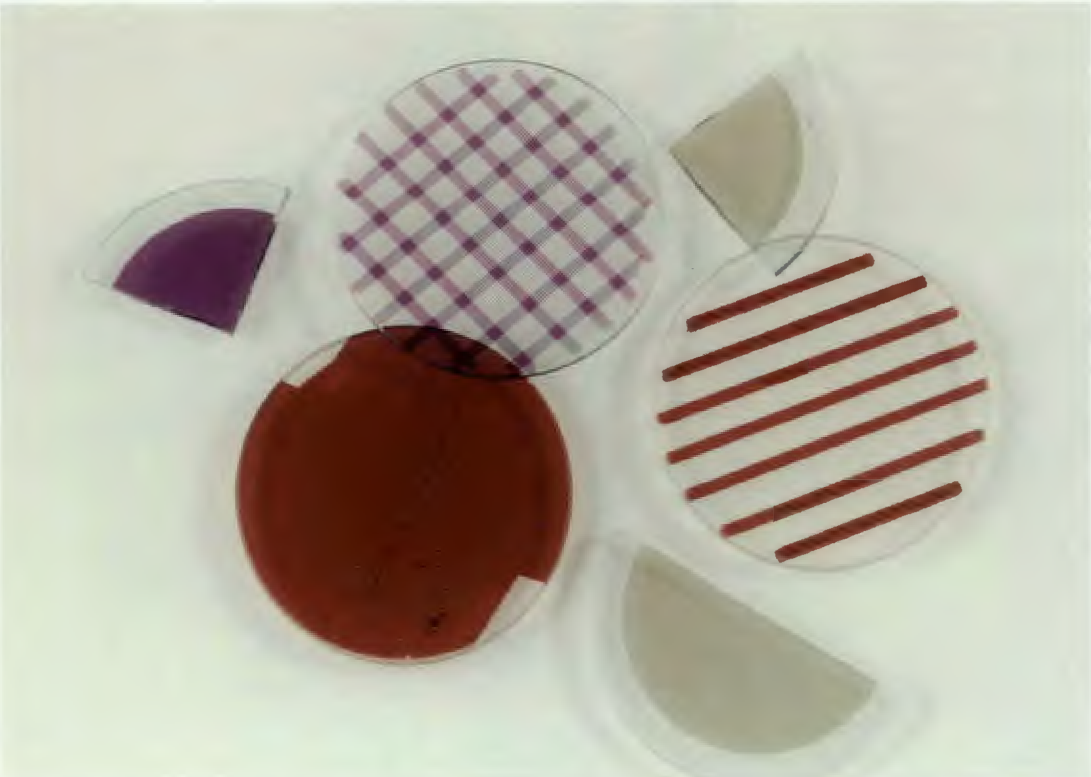
Nanocrystal properties have been exploited throughout the centuries. For example, since the Middle Ages, glaziers experienced in the art of making stained glass have incorporated small metal precipitates in molten glass to produce vibrant colors. However, researchers are only now beginning to understand enough about such phenomena to predict and intentionally control the behavior of small clusters of atoms.

At ORNL, high-energy accelerators are used to implant metal ions, such as gold, into silica (SiO_2), one common type of glass. The surface region of gold-implanted silica is much more supersaturated with metal atoms than silica treated by conventional techniques. During high-temperature annealing, gold nanocrystals approximately 10 nm in diameter are formed by precipitation. In addition to their striking colors (shown in the photograph below), such ion-implanted samples reveal many other useful optical properties, such as a refractive index that depends strongly on the intensity of light striking the material.

Scientific and technological interest in nanocrystals extends far beyond stained glass. ORNL researchers have shown that ion implantation can be used in a novel way to create high densities of a wide range of nanocrystals in a number of technologically important materials, including silica, sapphire (Al_2O_3), and even crystalline silicon. In this approach, high-dose ion implantation of the near-surface region creates a solid solution that is supersaturated with impurity ions. When the sample is heated, the highly concentrated impurity ions precipitate out, forming nanocrystals that usually cannot be synthesized by conventional methods.

The objective of this research is to understand and control the size, structure, and optical and physical properties of nanocrystalline composites produced by high-dose ion implantation. In addition to the metallic nanocrystals

Ion beams synthesize nanocrystals, forming light-emitting materials and compound semiconductors.



Striking colors arise from gold nanocrystals formed in sapphire and fused silica by ion implantation. Encapsulated gold nanocrystals produce purple or red.

shown in the photograph, ORNL researchers have demonstrated that elemental semiconductor nanocrystals of silicon and germanium can be synthesized in SiO_2 and Al_2O_3.

We have observed a strong red light from SiO_2 samples containing silicon nanocrystals. The light intensity is comparable with that from porous silicon, and the wavelength (i.e., color) can be tuned by changing nanocrystal size. Because size determines the wavelength of emitted light, full-color panel displays for computers may someday be made of appropriately sized semiconductor nanocrystals formed by ion implantation.

The researchers have also synthesized more complex compound semiconductors and alloy nanocrystals (e.g., silicon germanium, gallium arsenide, cadmium selenide, and gallium nitride) by implanting combinations of different ions into silica and sapphire hosts. By controlling implantation and annealing conditions, they discovered that it is possible to control orientation and, in some cases, crystal structure of nanocrystals.

The scientists also incorporated compound semiconductor nanocrystals such as gallium arsenide (GaAs) into a silicon matrix. The optical properties of this nanocrystalline composite are expected to be considerably different from those of current silicon-based devices because energetic electrons can be directly converted into visible light in GaAs, but not in silicon. It may be possible to produce buried continuous layers of GaAs by extending ion implantation to higher doses. This approach could provide a way to combine silicon-integrated circuits with high-speed GaAs layers to achieve fully integrated optoelectronic devices.

This research provides a new way to form encapsulated nanocrystals in materials to investigate the nanocrystals' size-dependent properties. The synthesis of a wide range of nanocrystals of various sizes in technologically important host materials should give rise to even smarter computers, as well as new electronic and optical devices never dreamed of by makers of stained glass windows.

This research was supported by DOE, Office of Energy Research, Basic Energy Sciences.

New Research Building and Laser MBE Film Growth

Brick by brick, a new building for ORNL's Solid State Division was constructed in 1995. Now, researchers in Building 3150 are using a pair of new laser molecular beam epitaxy (MBE) systems to build novel materials, atomic layer by atomic layer. Dedicated September 15, 1995, Building 3150's second floor houses the laser MBE systems that are used to synthesize new crystalline thin-film materials for electronic and photonic uses, as well as facilities for semiconductor processing, supersonic-jet film growth, and photolithography.

The two laser MBE systems developed at ORNL are being used to grow thin films on single-crystal substrates in a controlled way near the atomic level. As in conventional pulsed laser ablation film growth, laser MBE films are grown in a vacuum or at very low pressures. A pulsed excimer ultraviolet laser beam vaporizes pressed polycrystalline targets containing mixtures of different elements, such as yttrium, barium, strontium, and copper. The vapors deposit as a film on a heated crystalline substrate that acts as an atomic-scale template to align the film's crystal structure.

ORNL's new laser MBE systems offer two advantages over conventional laser ablation equipment: better control of growth at the atomic

The Solid State Division's Building 3150 under construction in 1995.

New laser molecular beam epitaxy systems in a new research building should produce better semiconducting and superconducting materials and greater understanding of their properties.

ORNL Director Alvin Trivelpiece (center), Associate Director Bill Appleton (right), and researcher Doug Lowndes admire new laser molecular beam epitaxy equipment in the Solid State Division's new building. *Photograph by Curtis Boles.*

level and a cleaner environment for growing highly pure crystalline films. Improved control is achieved through new capabilities. Now, it's possible to "tune" energies of incident atoms and ions, control substrate temperature from below room temperature to 900°C, and rotate the substrate to make film thickness and composition more uniform. ORNL is developing a new type of ellipsometer that will monitor film thickness and optical properties during film growth in gaseous environments, where conventional electron beam monitoring cannot be used. The laser MBE system also provides auxiliary evaporation, ion beam, and plasma sources to assist film growth and doping. The clean, ultrahigh-vacuum-growth environment ensures that very few water vapor or other unwanted gas molecules will be present to contaminate the product.

One laser MBE system will be used to grow semiconducting films that contain several different chemical elements (e.g., zinc selenide telluride alloys or copper indium gallium diselenide) and to dope them with deliberately added impurity atoms. The goal: improve the films' electrical, light-emitting, and light-absorbing properties and better understand the physics underlying the improved properties. Applications for such materials include photovoltaic cells for converting solar energy to electricity, flat panel displays to replace bulky computer monitors, higher-density data storage for compact disc players and computers, and perhaps optical computers.

Another laser MBE system is being used to build and study thin films of artificially layered high-temperature superconducting materials. The goal of these experiments is to provide basic data that will allow researchers to relate systematic variations in film structure and composition to changes in their superconducting properties.

While the new laser MBE growth systems were being developed, ORNL researchers used conventional laser ablation growth chambers to simulate and investigate several capabilities of laser MBE. For example, in 1994 they grew "superlattice" structures consisting of alternating strontium-copper-oxide and barium-copper-oxide layers to form two new families of superconductors that do not exist as bulk materials. These new, artificial thin-film superconductors, built of sheets of copper oxide, were shown to be high-temperature superconductors (with superconductivity observed at temperatures as high as 70 Kelvin). The work was reported in *Science* magazine. In 1995, the growth of highly doped (electrically conducting) zinc telluride semiconductor films was achieved by another group of ORNL researchers and reported in *Applied Physics Letters*.

The improved capabilities of the new laser MBE systems should make possible even better semiconducting and superconducting materials and greater understanding of their properties. Consequently, ORNL's new research building and laser MBE facilities are expected to help our solid-state physicists build on their previous successes, bit by bit.

The building and new instruments were made possible with funding from DOE, Office of Energy Research, Basic Energy Sciences.

Automotive Catalyst Atoms Observed

Precious metals on a ceramic are helping cars clean up their act. A sprinkling of silvery-white platinum or rhodium atoms on gamma alumina "supports" in catalytic converters can increase the rate of important reactions: oxidizing the major pollutants of auto exhaust—nitrogen oxides, carbon monoxide, and hydrocarbons—to harmless nitrogen, carbon dioxide, and water.

No one understands precisely how platinum and rhodium work as catalysts in cars, but use of ORNL-developed Z-contrast microscopy (see images on p. 60) is providing the first atomic-scale glimpse of these important materials. Now, we can see where and how metal atoms sit on the ceramic surface and relate this information to peaking or fading of catalytic action, which chemists measure by passing test gases over catalytic converter materials.

Using a 300-kilovolt scanning transmission electron microscope, we can easily distinguish the heavier catalytic metal atoms from our substrate's lighter atoms of aluminum and oxygen (atoms of higher mass appear much brighter in the image). We observed the structure of small clusters of metal atoms that sit on top of each other like a cheerleader pyramid and reconstructed their three-dimensional form. For platinum, we imaged a mixture of single metal atoms and scattered triplets. For rhodium, we observed numerous 1-atom-thick "rafts," each about 6 to 10 atoms wide (like a cluster of islands in a bay).

Rhodium is now being used more than platinum as an automotive catalyst because it can promote the oxidation of three major pollutants. Unfortunately, it is less stable, and the mechanism responsible for its degradation is not well understood. We have observed an atomic-scale mechanism that can explain the catalyst's degradation: clusters of rhodium atoms diffuse into vacancies that are naturally present in the gamma alumina lattice.

If funding is available through collaboration with the automobile industry, we hope to conduct more research to identify the active sites of the catalyst metal atoms and the chemical reactions they promote. Because rhodium is so expensive, it would be desirable to maximize its efficiency and minimize its degradation, to make catalytic converters effective for the long haul. Alternatively, a less expensive metal could perhaps be made to work as well. Our studies could help the auto industry and government nail down this information as they act together to design a clean, efficient, and affordable car.

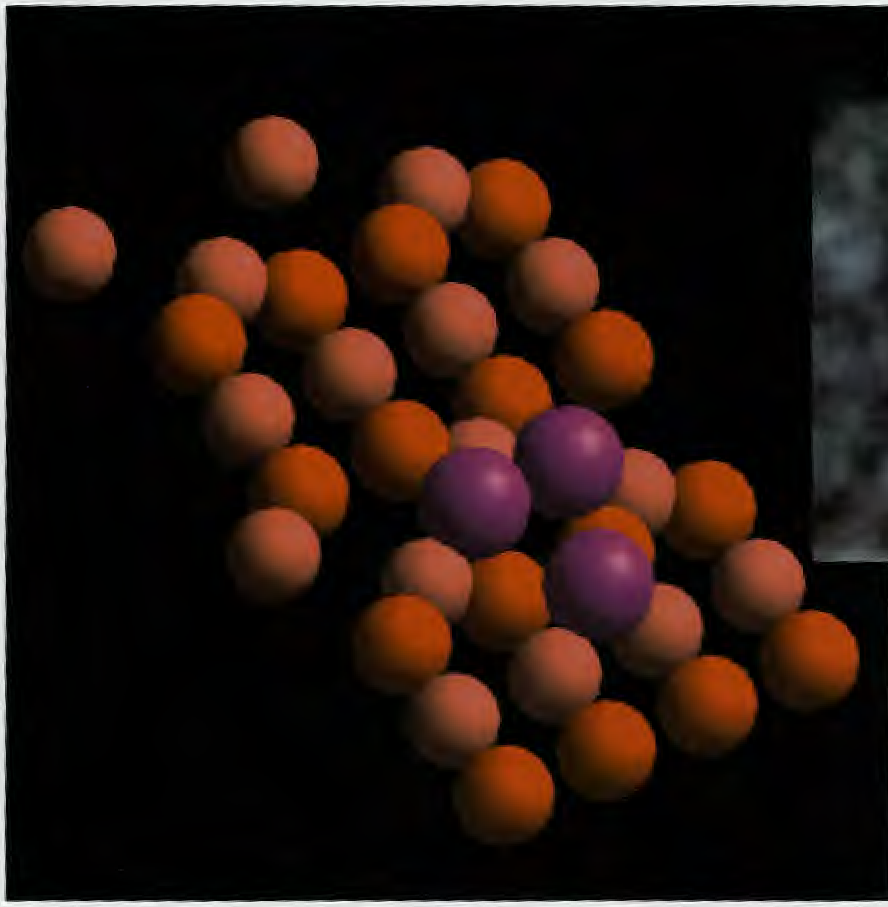
The research was supported by ORNL's Laboratory Directed Research and Development Fund.

Linking Welding Process with Weld Properties

ORNL's welding and joining researchers have been making connections—between the welding process and weld microstructure and properties and with scientific and industrial experts. As a result, our group is setting trends in welding research and development. We are internationally known as the leader in understanding and predicting relationships between weld microstructure and properties.

A stainless-steel weld has a microstructure that gives rise to properties such as strength and toughness. When a weld is exposed to high temperatures over a long time, its microstructure changes, often making it brittle. Brittle welds have forced costly shutdowns of petrochemical and power plants.

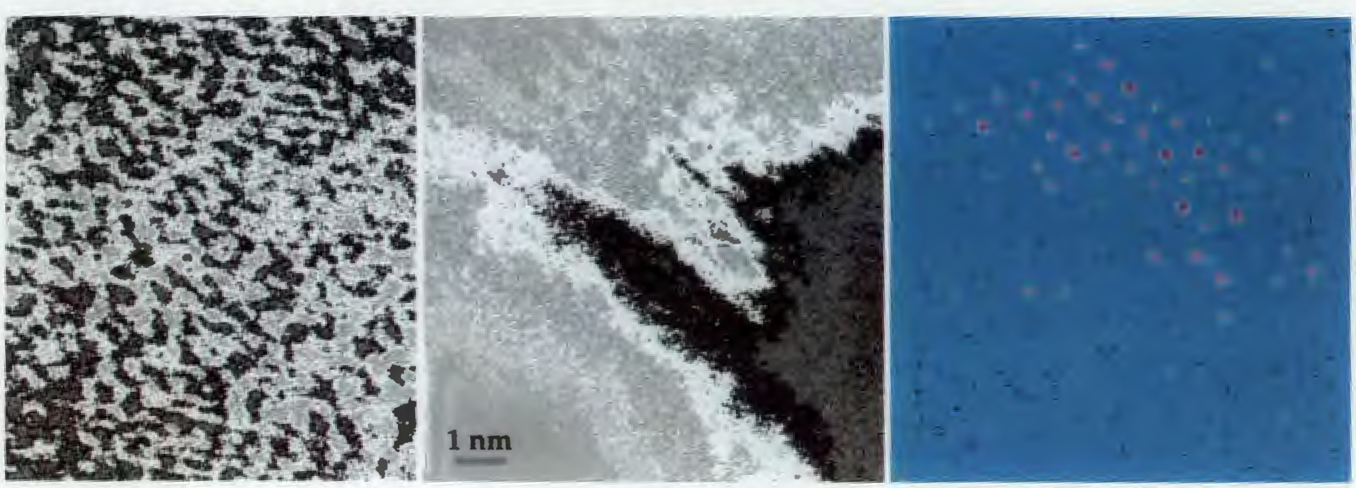
We have provided basic information on the aspects of microstructure that control fracture toughness in austenitic stainless-steel welds at low temperatures. Our research goals are to



Z-contrast image (inset) of a platinum catalyst on gamma alumina (γAl_2O_3) showing individual atoms arranged as trimers. From such data the likely adsorption sites of platinum atoms (three purple balls) on the alumina surface can be determined, as seen in the simulation.

Thanks to Z-contrast microscopy, we can explain degradation in an automotive catalyst at the atomic level.

Images of a rhodium catalyst supported on gamma alumina taken with the 300 kilovolt scanning transmission electron microscope. In the phase contrast high resolution image (left), the type of image normally taken with conventional microscopes, the rhodium is invisible. However, the rhodium atoms are seen clearly in the Z-contrast image (center) and in pink in the colorized form (right). The arrangement of the rhodium atoms corresponds to no known form of metal or oxide, but does correspond to normally vacant atomic sites in the alumina. The rhodium is thought to have dissolved into these normally empty sites, where it will no longer be catalytically active. This image reveals clearly for the first time how a catalyst can lose its activity through aging, limiting its automotive applications.



We find and predict relationships between the welding process and weld microstructure and properties.

Ripples, or surface undulations, are formed during the stationary arc welding of a single crystal of austenitic stainless steel, as shown in this interference-contrast micrograph.

determine desirable microstructures for different weld materials, predict properties of weld microstructures transformed by heat over time, and develop intelligent automated techniques for controlling the welding process, to obtain welds that give the best properties.

Using data from our experiments with single-crystal stainless-steel welds, we have developed analytical and computational models that describe relationships between the welding process and microstructure of welds. Applying this knowledge, we have been working with Westinghouse Electric Corporation on ways to repair gas-turbine-engine components made of single-crystal, nickel-based superalloys. These components are critical to the operation of turbine engines in jet aircraft and power plants.

We are also studying the role of oxide inclusions in improving or degrading properties of steel welds. Oxygen that has been dissolved in molten steel forms oxide inclusions with the steel's residual elements, such as aluminum, manganese, silicon, and titanium. As the steel cools and solidifies, these oxide inclusions are frozen into the microstructure. If a steel weld has the "right" number and distribution of oxides and the "right" overall composition, the weld will contain good microstructural constituents that would make the weld tough. If not, it may have poor mechanical properties. We have developed a model to predict a weld's inclusion characteristics and microstructure based on oxide inclusion composition, number density, and size distribution.

We hope our knowledge of welding can be applied to the design of lightweight, efficient cars built from aluminum parts for the Partnership for a New Generation of Vehicles. In the meantime, our group has received new recognition: The Institute of Materials in London, England, has founded the first scholarly journal in the field—*Science and Technology of Welding and Joining*—and named ORNL's Stan David the inaugural editor-in-chief. To advance welding research, we hope to continue to make the right multidisciplinary connections.

The research is sponsored by DOE, Office of Energy Research, Division of Materials Sciences.

Improving Auto Brakes With Neutrons

You're driving a Ford Taurus when a car veers into your lane. You slam on the brakes, stopping in time and avoiding a collision. As usual, the brakes are reliable, but because they vibrated that time, you take the car to the dealer to have them checked.

You're told these vibrations are more annoying than serious. But because service personnel frequently must deal with the problem, one of the Ford Motor Company's goals is to reduce the costs of servicing brakes—to the company and the owner—over the lifetime of each vehicle.

To help accomplish this goal, Ford researchers conducted studies at ORNL's Residual Stress User Center. This center provides neutrons and X rays to probe materials for residual stresses—internal stresses that develop and remain in a material as a result of manufacturing and other forces. The Ford researchers wanted to better understand the effect of residual stresses on disc brake rotors. These discs spin when the car moves until brakes are applied, hydraulically pressing pads against the discs to slow or stop them—and the car.

It was believed that when disc brake rotors overheated, changes in residual stresses in the discs caused them to distort, prompting vibrations during braking. The researchers wanted to know if heat treatment of rotors would reduce distortions and the probability of vibrations.

The Ford researchers brought to ORNL a standard rotor for measurement. They then heat treated it and brought it back to ORNL for comparison measurements. The goal was to determine the relief of stresses by heat treatment. The residual stresses in the rotors were mapped using neutron diffraction at our HFIR. Residual stresses cause distances between planes of atoms in a crystalline material to shrink or stretch compared with normal lattice spacings in stress-free areas. Because varying distances between atomic planes affect the angles at which neutrons are diffracted or scattered, lattice strains resulting from residual stresses can be precisely located and measured.

The Ford Motor Company analyzes brake rotors at ORNL's Residual Stress User Center.

Bill Donlan, a Ford Motor Company researcher, prepares to use neutrons from ORNL's High Flux Isotope Reactor to map residual stresses in automobile brake discs. *Photograph by J.W. Nave.*

Neutron stress mapping studies showed that standard rotors have significant stresses that can be reduced by heat treatment. The data should help Ford modify the brake manufacturing process. Ford may soon be putting a stop to stresses that could affect brakes—and drivers.

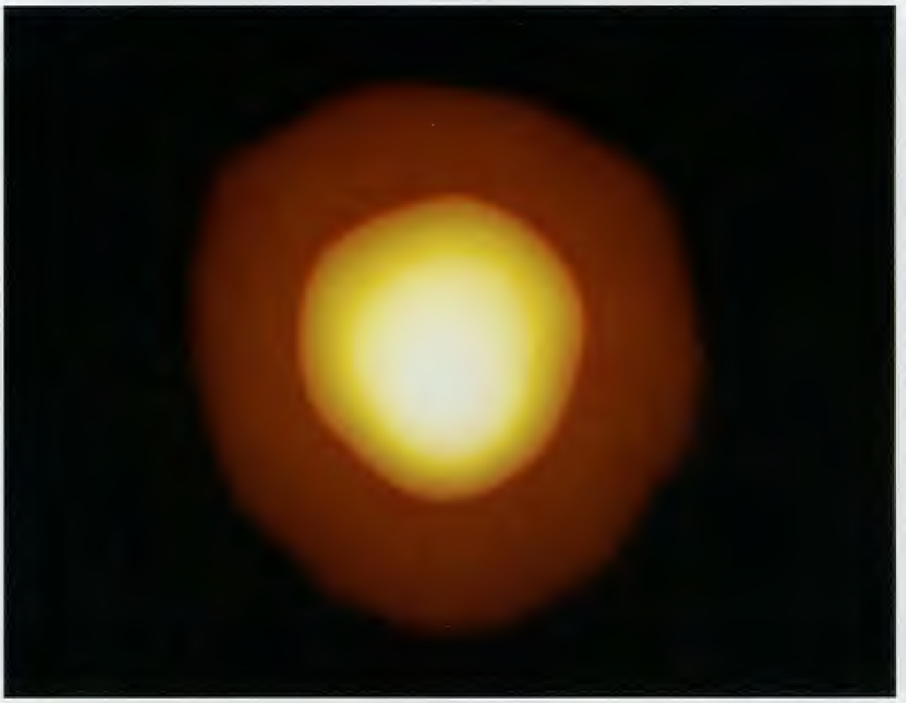
The research is sponsored by DOE's Office of Energy Efficiency and Renewable Energy, Office of Transportation Technologies, as part of the High Temperature Materials Laboratory User Program. The High Flux Isotope Reactor is sponsored by DOE's Office of Energy Research. ornl

Physical Sciences

ORNL physicists in the Physics Division investigate fundamental properties of matter at the atomic, nuclear, and subnuclear level. They develop experimental devices in support of studies in atomic, nuclear, and high-energy physics. ♦ The Physics Division operates four experimental facilities: the Oak Ridge Electron Linear Accelerator, used to measure neutron cross sections to help resolve issues in nuclear astrophysics; the Holifield Radioactive Ion Beam Facility (HRIBF), which is being prepared for the first experiments using radioactive ion beams later this year; the EN-Tandem Accelerator, and the recently upgraded Electron Cyclotron Resonance Ion Source Facility. The latter two are operated in support of the atomic physics research community. ♦ The experimental nuclear physics program emphasizes use of heavy ions to probe the structure of heavy nuclei and address questions in nuclear astrophysics. Our physicists conduct their research here and at accelerator facilities around the world, including the Super Proton Synchrotron at the European Laboratory for Particle Physics (CERN). ♦ Atomic physicists conduct channeling and energy-loss experiments, study charge change in projectile beams at ultrarelativistic energies, and perform research in support of the fusion energy program. Theoretical physicists work in support of experimental physics to predict outcomes and better understand results. ♦ In the Solid State Division, physicists seek to understand properties and interactions of a wide range of materials for possible use in advanced energy technologies, such as thin-film batteries and semiconducting and superconducting materials. By studying interaction of particle beams with materials, they develop new materials and materials processing techniques (see pp. 56 to 59 for highlights on the materials research of our solid-state physicists). Physical sciences also includes chemistry. Several of our scientists are geochemists (see pp. 68 to 69) who explore phenomena within the earth while some of our nuclear physicists look beyond it.

Probing the Evolution of Stars

ORELA sheds light on the synthesis of elements in the universe and other puzzles in nuclear astrophysics.



Red giant stars are responsible for producing many of the heavy elements. Measurements at ORELA play an important role in furthering our understanding of how those elements are produced.

Neutrons produced at the Oak Ridge Electron Linear Accelerator (ORELA) are helping ORNL's star shine in the astrophysics community. ORELA, which produces energetic bursts of neutrons by bombarding a tantalum target with electrons, has already been used to measure 180 neutron cross sections of astrophysical significance. These data are important to our understanding of how elements heavier than iron are slowly synthesized in stars by a series of neutron captures known as the s-process.

In four billion years, our sun will become a red giant—a bright, bulging star that will have cooled to a low temperature. Similar stars are believed to have produced many of the heavy elements in the universe. Nuclear reactions in these stars can produce large numbers of neutrons that are later captured by iron "seed" nuclei to form elements as heavy as bismuth. ORELA has supplied much of the nuclear data needed to understand the s-process. However, it was recently learned that the s-process may be occuring at a temperature three times lower than previously believed. Because more nuclear data are needed to understand effects of a lower temperature on the s-process, ORELA is again supplying this information. ORNL physicists have recently measured neutron cross sections on two key elements: barium and neodymium. Measurements of other cross sections important for understanding heavy element production are also under way.

Our physicists are also using ORELA to address other puzzles in nuclear astrophysics. A recent ORELA measurement addresses how light elements were formed during the Big Bang. The standard Big Bang model, which assumes that matter was uniformly distributed in the early universe, suggests that no elements heavier than lithium were formed until after the birth of stars. However, in Big Bang models that assume that matter existed in clumps, it may be possible to synthesize elements such as carbon, nitrogen, and oxygen in very neutron-rich regions.

In a study of a crucial link in a sequence of nuclear reactions that could form heavier elements in a clumpy universe, ORNL physicists measured the probability that lithium-7 nuclei in a target would capture neutrons from ORELA, forming lithium-8 and emitting detectable gamma rays. Their results, which help resolve discrepancies among previous measurements of this reaction, suggest that carbon may have been formed before stars were born. If these isotopes thought to be present in the early universe are observed by the Hubble Space Telescope, it may be possible to determine the "clumpiness" of the universe minutes after the Big Bang.

Another puzzle that was addressed in this measurement concerns the neutrinos produced by nuclear reactions in our sun. Solar neutrinos are the only direct probe of the nuclear reactions that power the sun. The problem is that 2 to 5 times more solar neutrinos have been predicted than detected. This discrepancy has led scientists to speculate that some neutrinos change to a different type of neutrino which cannot be detected in many experiments. However, the number of neutrinos detected in most experiments is very sensitive to the rate of fusion of protons with beryllium-7 in the sun. This reaction will be studied directly in a future experiment at the Holifield Radioactive Ion Beam Facility using a radioactive beryllium-7 beam, but the ORELA lithium-7 experiment also sheds light on this reaction.

The fusion rate of the proton/beryllium-7 reaction is determined using a theoretical model that predicts that fusion occurs only in "head-on collisions." A recent Duke University study of a similar reaction suggests this may not be the case. The ORELA experiment is relevant because the lithium-7 reaction with neutrons

At CERN we found no evidence to rule out the existence of free quarks right after the universe's birth.

"mirrors" the beryllium-7 reaction with protons. In the ORELA experiment, no evidence of fusion was seen in collisions other than head-on ones, supporting the standard theoretical model. ORELA continues to offer shining examples of its benefits to the astrophysics community.

The research has been supported by DOE, Office of Energy Research, Office of High Energy and Nuclear Physics.

Closing in on First Moments of the Big Bang

Re-creating the first ten microseconds of the Big Bang requires a big boost in accelerator beam energy. ORNL physicists working with an international team have been searching for the primordial soup of the early universe using ultrarelativistic beam energies 10,000 times those obtained at ORNL's Holifield Heavy Ion Research Facility. Since 1986 their hunting ground has been the Super Proton Synchroton of the European Laboratory for Particle Physics (CERN). In 1999 they will begin a series of experiments at the Relativistic Heavy Ion Collider (RHIC) at DOE's Brookhaven National Laboratory.

Some 15 billion years ago, an infinitely compact, superdense particle hotter than 1500 billion kelvins began to expand and cool rapidly in what is called the Big Bang. After a few microseconds of cooling, vast amounts of energy were partially converted to particles of matter—free quarks and gluons, leptons (such as electrons), and photons. By the tenth microsecond, this quark-gluon plasma condensed into the known particles that form the nuclei of atoms. Quarks are the basic constituents of protons and neutrons in atomic nuclei, and gluons are the force-carrying particles that bind quarks together.

Quarks have never been observed in a free, unconfined state. They prefer to exist only in quark-antiquark pairs (mesons) or quark triplets (protons and neutrons). The goal of the CERN experiments has been to show that free quarks can be produced and detected by "boiling" them out of protons like a yolk bursting from the shell of a microwaved egg. To heat protons enough so that the quarks would slam together and break out of the proton "skins," nuclei of oxygen, sulfur, and lead were stripped of all electrons, accelerated, and collided in different experiments with target nuclei of carbon, copper, silver, and gold at ultrarelativistic energies of 32 trillion electron volts (99% the speed of light).

The experiments dramatically demonstrated the conversion of energy into matter; for example, a collision between nuclei of oxygen and gold involving initially only 87 charged particles (protons) sprayed out over 400 charged particles. But the experimenters were mostly interested in measuring emitted photons because they would signal the presence of free quarks. Because each quark has an electric charge, it will radiate a photon any time it changes direction after it breaks free. This experiment, however, has a complication: Any quark-antiquark pair formed in these collisions may recombine later into a neutral pi meson, which subsequently decays and emits two photons. Thus, lead-glass calorimeters containing over 10,000 pieces of glass were built by Russian researchers to detect the many photons. German scientists built instruments to calibrate the photon energies, and Oak Ridge researchers, who built calorimeters for the early CERN experiments, developed the electronics to distinguish between photon signals from quarks and those from pi mesons.

The international team increased energy density—internal energy of nuclei at rest—20 times, generating many more decay products; saw no evidence to rule out the existence of the quark-gluon plasma, and found no proof that deconfinement—the existence of lone quarks—did not occur. They also could set limits on how hot the resulting system must have been, finding temperatures about 100,000 times hotter than those at the core of the sun.

As the experiments are continued at RHIC to achieve even higher energy densities, our understanding of the conditions right after the universe was born should receive another big boost.

The research was supported by DOE, Office of Energy Research, Division of High Energy and Nuclear Physics, Office of Nuclear Physics.

CERN Results May Affect Collider Operation

Like two race cars careening around a circular racetrack in opposing directions, two beams of gold ions will smash into each other at a velocity greater than 99% the speed of light. At least that's one plan for the RHIC, now under construction at DOE's Brookhaven National Laboratory.

There may be a problem with this plan. ORNL atomic physicists in an international collaboration have observed an interesting effect when an ultrarelativistic beam of lead ions accelerated at 33.2 trillion electron volts strikes a thin gold target. During experiments at the Super Proton Synchrotron at the European Laboratory for Particle Physics (CERN) near Geneva, Switzerland, researchers from ORNL, Denmark, Germany, and Sweden noted a change in the lead ion beam that stemmed from a dramatic conversion of energy to matter. All the lead ions had been fully stripped of electrons before they were accelerated toward the target, but at the time of impact, up to 0.1% of the lead ions each picked up an electron. Where did these electrons come from?

When a lead projectile collides with a target nucleus, the electric field of the two nuclei is so strong that a virtual photon arises, generating at least one electron-positron pair. Because the lead ion has a strong positive charge, the pair's negatively charged electron may be captured in a lead electron shell while its positively charged mate, the positron, is repelled. The captured electron may be in the excited or ground state. The probability of electron capture was determined by measuring the rate at which lead ions emerging from the target changed their charge.

What are the implications for RHIC (and CERN's Large Hadron Collider, also under construction)? If colliding gold ions in one of two beams pick up electrons, the charge-to-mass ratio for which the accelerator ring magnets are tuned will change. Thus, the beam may crash into the wall, requiring a new beam to be introduced frequently into the ring. More electron-capture experiments are needed to determine if the desired efficiency and reliability of collider operation will require use of ion beams from lighter elements—not quite as good as gold.

We found that a few electronless lead ions in an ultrarelativistic beam picked up electrons at the target.

Herb Krause examines the beam line of the Super Proton Synchrotron at the European Laboratory for Particle Physics (CERN).

* * *

Another phenomenon studied by ORNL physicists at CERN was the ability of the target material to slow down ultrarelativistic projectile ions after impact—the so-called electronic stopping power. For lead ions on a lead target, a new theory that considers the effect of finite nuclear size calculates that the stopping power should be less than what the old theory concludes. Our physicists found that lead ions lose less energy in a lead target than the old theory predicted, validating the new theory for heavier elements. Energy losses for lighter target elements, such as carbon, were closer to those predicted by the old theory. The drive to do new experiments to help refine the theory has not stopped.

The research was supported by DOE, Office of Energy Research, Basic Energy Sciences, Office of Chemical Sciences.

ORNL Discovers Superdeformed Light Nuclei

Some nuclear physicists like them exotic—slender, not round. In their atom chase, they search for "superdeformed" nuclei that are twice as long as they are wide. These atomic cores are different from normal baseball-shaped nuclei because, for a split second, they look like footballs.

In the 1960s, it was discovered experimentally that nuclei of heavy atoms such as plutonium-240 and other actinides assume elongated shapes and have a good chance to fission spontaneously into two fragments. So theorists proposed that rapidly rotating nuclei of certain groups of lighter elements could take on the same football shape. Subsequent calculations identified groups most likely to show this effect—some elements with atomic masses of 190 to 210, 150 to 160, and 80 to 90.

In 1986 the first experimental evidence of a superdeformed shape in a nucleus outside the actinide group was observed in dysprosium-152. In 1989 a similar shape was seen in mercury-192. But until recently, the race by many research groups to catch a glimpse of nuclear footballs in the mass 80 to 90 range went on without success. The physicists in pursuit hailed from Denmark, England, France, Germany, Japan, and the United States, including a group at Oak Ridge.

The ORNL physicists' first hunting ground was a tandem accelerator at

Daresbury Laboratory in England. There, in 1993, they discovered the first light-mass superdeformed nucleus in strontium-83. Since then, they have continued their search at DOE's Lawrence Berkeley National Laboratory (LBNL), where they take advantage of the Gammasphere, the world's most sensitive gamma-ray detector system.

The nuclei of interest are typically synthesized by bombarding a nickel-58 target with beams of silicon-28 or sulfur-32 ions. Occasionally, some ions strike the target nucleus nearly head-on and fuse with it with little spin. But many ions hit the target nucleus off center and produce fused compound nuclei that rotate very rapidly. As a spinning nucleus drops down from its excited state, it releases its excess energy, first by emitting particles (neutrons, protons, alpha particles) and then gamma rays. The gamma rays are particularly effective in carrying away the excess energy of rotation.

In superdeformed nuclei, the gamma-ray energies drop with decreasing spin in a very regular fashion. The regularity of the energies of these gamma rays and the time it takes for the nucleus to emit them are used by physicists to determine how deformed these nuclei are. Their measurements of lifetimes of these superdeformed states indicate that, unlike toy gyroscopes, these fast-rotating nuclear tops last for a mere 10^{-15} to 10^{-13} seconds before they jump to their next lower state.

By now, the ORNL group and collaborators from Washington University, LBNL, the University of Pittsburgh, and Florida State University have detected more than 10 cases of superdeformed nuclei that have masses in the range of 80 to 90 and span four different elements: strontium, yttrium, zirconium, and niobium. Rotating at the rate of about 10^{22} turns a second, they are the fastest-spinning nuclei yet observed. The measured properties of these nuclei are in reasonable agreement with the predictions of theory, but some puzzles remain. The race is on to find the solutions.

We've detected short-lived, football-shaped nuclei of strontium, yttrium, zirconium, and niobium.

This rapidly spinning nucleus has assumed the "superdeformed" shape—it is twice as long as it is wide, like a football.

The research is supported by DOE's Office of Energy Research, Office of High Energy and Nuclear Physics.

Gamma Rays Speed HFIR's Embrittlement

In November 1986, ORNL's High Flux Isotope Reactor (HFIR) was temporarily shut down because its vessel was found to be undergoing a higher than expected rate of embrittlement. Neutron radiation was initially blamed. ORNL scientists now believe that gamma rays, which were not previously suspected, are responsible for the unusual embrittlement.

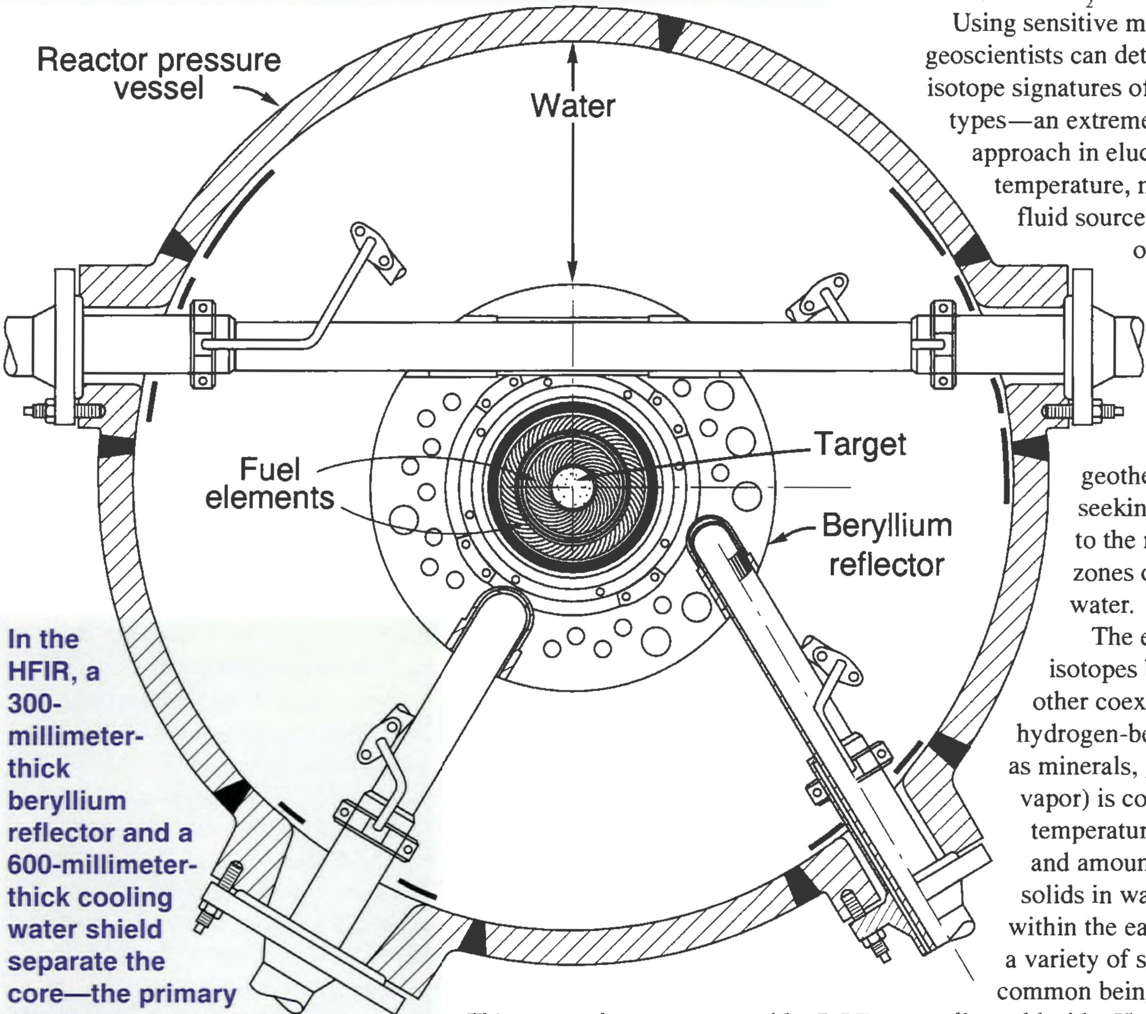
All nuclear reactor vessels experience radiation-induced loss of ductility, or embrittlement. The main reason: fast, or high-energy, neutrons collide with atoms of the vessel material, knocking them out of their regular positions, creating tiny point defects. Some point defects crowd together into clusters that harden the metal and make it less ductile.

The significance of gamma rays to the HFIR vessel embrittlement was discovered when beryllium and neptunium-237 monitors were used to verify the fluxes of fast neutrons—the number of neutrons striking a certain area per second—at vessel surveillance positions. These monitors seemed to indicate a much greater fast-neutron flux than did the regular iron and nickel monitors. This discrepancy was traced to interference from gamma rays. Beryllium and neptunium-237 are sensitive to both fast neutrons and high-energy gamma rays, whereas iron and nickel monitors are unaffected by gamma rays. The ratio of gamma flux to fast neutron flux was found to exceed 1000 to 1. It was realized that this exceptionally large ratio could explain the extra embrittlement of the vessel.

Although gamma rays have insufficient momentum to directly dislodge an atom in steel, they can energize the steel's electrons, which can displace atoms. It takes more than 1000 high-energy gamma rays to create the same number of atomic displacements as a single fast neutron. However, for a ratio greater than 1000:1, the gamma-induced atomic displacements will make a larger contribution to embrittlement than will the fast neutrons. Thus, gamma irradiation accounts for the hitherto puzzling rapid embrittlement of the HFIR vessel.

The HFIR case is the first known example of reactor pressure vessel embrittlement dominated by gamma irradiation. The reason lies in the design of the reactor. A 300-millimeter-thick beryllium reflector and a 600-millimeter-thick cooling water shield separate the core, the

Gamma rays, not neutrons, were found to induce the HFIR vessel's unusual rate of embrittlement.



In the HFIR, a 300-millimeter-thick beryllium reflector and a 600-millimeter-thick cooling water shield separate the core—the primary source of high-energy gamma rays and neutrons—from the vessel. These features block the flow of most neutrons, not gamma rays.

primary source of high-energy gamma rays and neutrons, from the vessel. Although these features present an effective barrier to most of the neutrons, they do little to deter gamma rays. Consequently, more than 1000 times as many gamma rays as neutrons strike the vessel wall.

Commercial nuclear power reactors have no beryllium and a much narrower water path, resulting in only a small ratio of gamma-to-neutron flux at the vessel and little or no embrittlement from gamma rays. The effects of gamma rays on the HFIR vessel are now being addressed in predictions of the vessel's lifetime.

This research was supported by DOE, Office of Energy Research, Division of Materials Sciences, and the Nuclear Regulatory Commission.

Pinning Down Isotope Signatures in Geological Samples

The waters in the oceans, rivers, lakes, groundwater, and fluids deep within the earth are different; each water has its own distinctive stable isotopic signature. The H_2O water molecules in a sample carry a special distribution of common light isotopes and rare heavy isotopes of hydrogen (deuterium, or D) and common oxygen-16 and rare oxygen-18 isotopes. Thus, the sample can include various minor amounts of $DH^{16}O$, $DH^{18}O$, and $H_2{}^{18}O$ molecules, as well as the common $H_2{}^{16}O$.

Using sensitive mass spectrometers, geoscientists can determine the stable isotope signatures of the various water types—an extremely powerful approach in elucidating the temperature, material fluxes, fluid sources, and time scales of ancient and active fluid-rock interaction processes in the earth's crust. Information of this sort can guide geothermal energy firms seeking to drill new wells to the most productive zones of steam or hot water.

The exchange of isotopes between water and other coexisting oxygen- or hydrogen-bearing phases (such as minerals, gases, or water vapor) is controlled by temperature and by the type and amount of dissolved solids in water. Fluids on and within the earth's crust contain a variety of salts, the most common being the familiar sodium chloride. However, ions in solution modify orientations of at least the nearest-neighbor water molecules relative to water as a whole to form an inner hydration shell. This rearrangement of water molecules in the vicinity of ions and the disruption of the hydrogen bonding network in the liquid lead to quite profound and quantifiable stable isotope redistributions. Until now, however, the influence of dissolved salts on stable isotopes in water has been largely ignored by the earth science community.

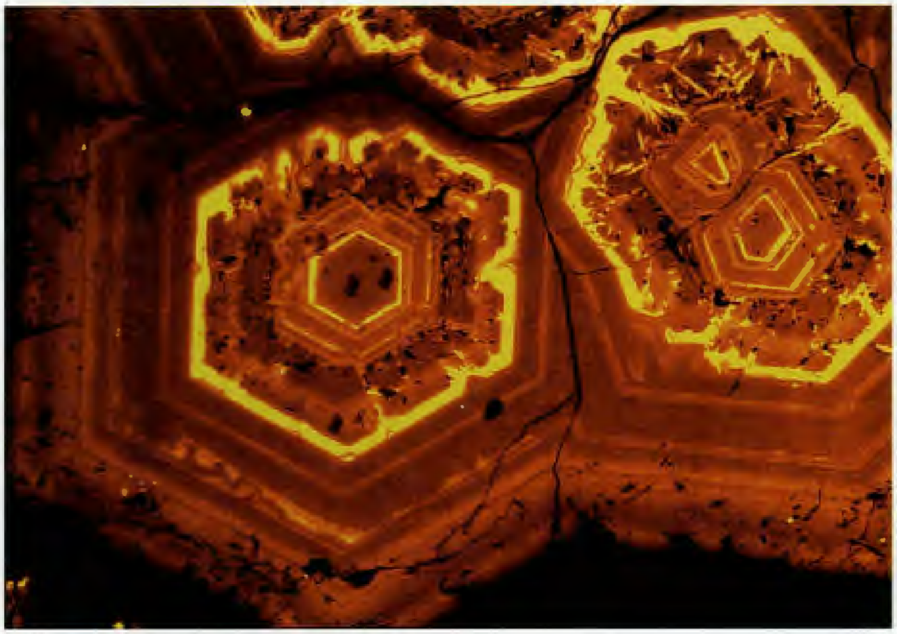
Our geochemists determined the effects of different concentrations of dissolved salts—sodium, potassium, calcium, magnesium chlorides, and sodium and magnesium sulfates—on the redistribution of oxygen and hydrogen isotopes between liquid water and water vapor as a function of

Our work on isotope ratios in underground samples guides geothermal energy development and understanding of the origins of sour gas in Canada.

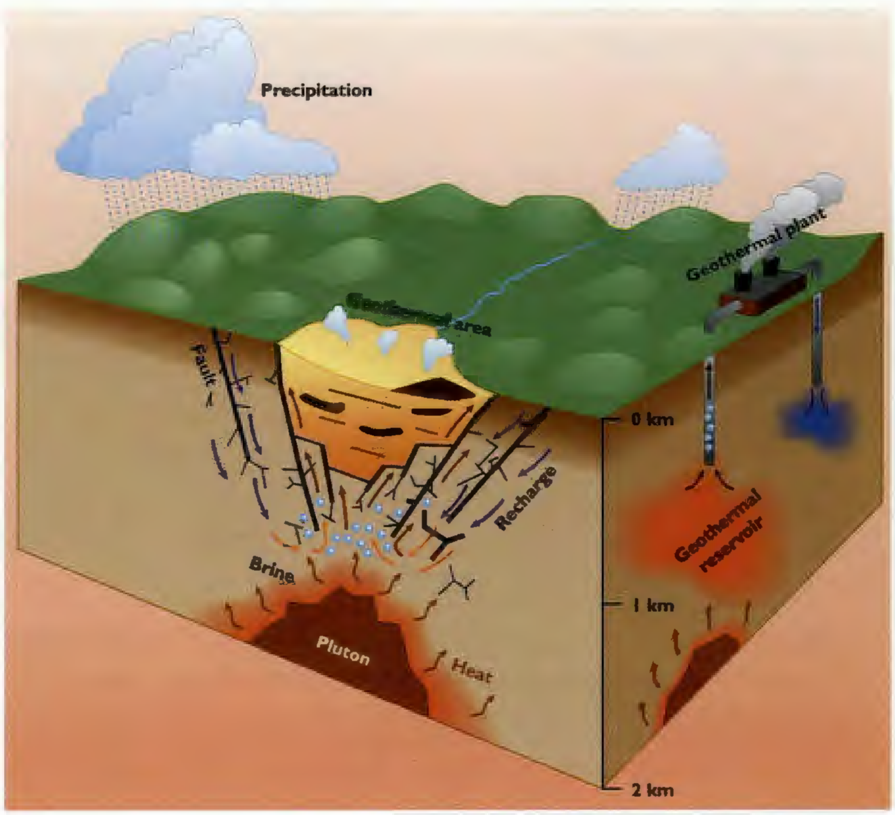
temperature. The magnitude of the isotope "salt effect" was found to increase with increasing temperature and concentration of the salt. From a practical point of view, data from this study have been used by the geothermal industry to understand the pressure-temperature-composition conditions of steam separation from brines both at the well head and in the subsurface-producing reservoir.

Traditionally, conventional stable isotopic analysis of geological materials involved manual separation of mineral samples and extraction of chemicals from homogenized powders. Thus, important spatial information, such as the temperature and timing of mineral formation provided by isotopic variations recorded in tiny mineral grains, was impossible to retrieve. Recently, our geoscientists have developed techniques to recover this information by using secondary ion mass spectrometry (ion microprobe) to measure intergrain and intragrain isotope ratios. Employing this technique to measure sulfur isotope ratios ($^{34}S/^{32}S$) at micron scales in pyrites, we discovered that the hydrogen sulfide that makes natural gas sour in western Canada does not originate from ancient bacterial metabolism of sulfate as once thought. Rather, we found that pyrite grains formed later in vast regions of sour-gas production are enriched in sulfur-34. This finding indicates that hydrogen sulfide was generated from thermal breakdown of sulfate by organic matter during deep burial of sediments associated with the building of the Canadian Rocky Mountains, some 60 million years ago. Through use of powerful tools, such as stable isotope geochemistry, our researchers are leaving their own distinctive mark in the geosciences field.

The research was sponsored by DOE's Office of Energy Research, Basic Energy Sciences, Geosciences and Chemical Sciences Divisions. ornl



Above is an image showing the relative amount of iron in an iron-calcium zoned mineral called a garnet. The intense, yellow bands are enriched in iron. Ion microprobe analysis provides information that can be used to interpret changes in the chemical environment as the garnet grew. Below are a geothermal system formed over a pluton heat source and a power plant that extracts energy from underground reserves of steam and hot water. *Illustration by Dave Cottrell.*



Computational Science and Advanced Computing

Computational science adds a new dimension to the more traditional experimental and theoretical approaches to scientific research. The use of computational tools has become vital to most fields of science and engineering and to many parts of the educational enterprise.

High-speed, large-scale computation has become the primary technology enabling advanced research in many areas of science and engineering. For this reason, blue-ribbon panels studying U.S. technological competitiveness have emphasized the critical importance of furthering our nation's traditional lead in high-performance computing technology.

Indeed, in many applications of interest to DOE and ORNL, computer simulations are the only feasible method of scientific investigation. Conventional methods would require prohibitively expensive experimental facilities and decades of effort. Leadership in this area requires the capacity to integrate advanced mathematical and computational techniques, data management and analysis methods, software tools, communications technologies, and high-performance computing systems.

At ORNL, we focus our strengths on scientific Grand Challenges and other highly complex computing issues. How? We integrate expertise in basic and applied research with the outstanding high-performance computing systems and infrastructure of our Center for Computational Sciences. Our strengths range from the ability to develop realistic mathematical models of complex phenomena and scalable algorithms for their solution to the availability of massively parallel processors and storage systems accessed by high-performance computing environments.

ORNL has long been a leader in computational plasma physics and materials science, nuclear physics and transport calculations, matrix computations, geographic information systems, and environmental information management. More recently, the Laboratory has become a leader in algorithms for parallel computers, informatics with emphasis on biosciences, global climate simulations, groundwater contaminant transport, distributed computing tools and interfaces, high-performance parallel computers, and data storage systems.

As a result of this leadership, we're working closely with major universities and with both computer and applications industries to conduct collaborative research and to commercialize technology. Automobile manufacturers, for example, are sponsoring computerized car-crash simulations at ORNL. And oil and aerospace companies are relying on ORNL's parallel virtual machine software to solve some of their most complex problems by linking many heterogeneous computers into high-performance, high-speed unified systems.

Our new software system enables our supercomputer to handle big and small jobs simultaneously.

Buddy Bland checks the operation of the Intel Paragon XP/S 150, a massively parallel computer at ORNL. *Photograph by Lynn Freeny.*

Speeding Up Access to the Paragon Supercomputer

Researchers seeking elusive answers to some very complex problems are now succeeding more quickly in Oak Ridge. A new software system developed for ORNL's Intel Paragon XP/S 150, one of the world's most powerful supercomputers, makes it possible for people doing more modest computing tasks and code development to work simultaneously with those performing huge production computing jobs.

Called overlapping partitions, the software system was designed by staff at ORNL's Center for Computational Sciences. The system was installed and demonstrated by Intel in January 1995 as the final milestone of a $16-million contract between ORNL and Intel Corporation. The new system allows users to simultaneously share the Paragon's 3072 parallel processors efficiently, automatically, and flexibly. Working together, these processors can perform 150 billion calculations per second.

Typically, researchers from around the nation use ORNL's supercomputer during the day in a "hands-on" fashion to work on codes and to perform a variety of computations—from relatively simple to elaborate. The Paragon performs these computations in seconds, minutes, or hours, depending on their complexity. Meanwhile, the computer also runs huge "production jobs," which require days, weeks, or months of computing time. These jobs include global climate modeling, studies of how solids melt, and simulations of magnetic alloys and nano-scale machines at the atomic level.

The new software allows quick access to the Paragon for these "hands-on" jobs without the need to stop longer-running production jobs. The overlapping partitions system frees the Paragon to perform calculations researchers need quickly during the day while simultaneously running the ongoing production jobs at various levels of capacity 24 hours a day, depending on priority and processor availability. This capability makes more efficient use of the computer's processors, allows more researchers to get computed results faster, and satisfies more customers. We can't always provide results as fast as the scientists wish, but we have taken an important step in the right direction.

Funding for the Center for Computational Sciences (CCS) at ORNL is provided by DOE's Mathematical, Information and

Computational Sciences Division and the Computer Hardware, Advanced Mathematics, and Model Physics (CHAMMP) Program for global change. Extensive information about the CCS, the Paragons, and overlapping partitions can be found on the World Wide Web at http:// www.ccs.ornl.gov.

Revolutionizing Science by Computer

You're a scientist and you want to simulate the synthesis of a new material on parallel computers rather than do time-consuming trial-and-error experiments in the lab. So you enter parameters such as how to mix the ingredients, when and how much to heat them and at what pressures, and when and how much to cool the molten material to strengthen it. Then you go home and rest while your simulation runs overnight. When you return the next morning, you're disappointed in the calculated results. You spend the next few days consulting with your collaborators and trying to figure out what went wrong.

Our CUMULVS software allows scientists to view and influence a simulated experiment in progress.

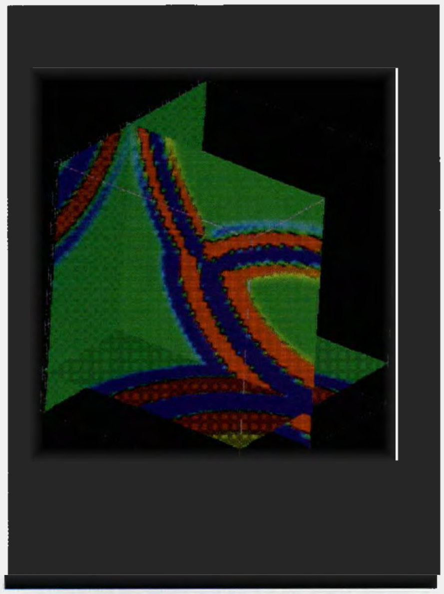


Image of a shock wave reflecting off an underground rock layer.

Things might have turned out differently if the same simulation had been augmented with the new ORNL-developed CUMULVS software system, named after cumulus clouds because collaborative environments and distributed computing are often depicted as a cloud. This system could revolutionize the way science is done by computers. CUMULVS was built to enhance collaboration and efficient simulation by allowing multiple scientists (possibly in remote locations) to view and influence the same simulation as it progresses. Each scientist can view the same or different aspects of the simulated process while it runs (interactive visualization) and can remotely change parameters to "steer" the process toward a desired result. For example, you might "see" that delaying the cooling of the molten material is weakening it, so you decide to interactively change the simulation to cool the material more quickly and see if it gets stronger.

CUMULVS also gives programmers the ability to protect their simulations from computer crashes—a critical capability when the simulation is executing in parallel across many computers. If requested, CUMULVS will save essential data (checkpointing) and automatically restart a failed component on a new computer (task migration).

Two large parallel applications have already incorporated the power of CUMULVS. An acoustic wave propagation simulation, which is of interest to oil exploration firms doing seismic analysis, models the transmission of sound waves traveling through and reflected by underground rocks of different densities. The second application aims at improving magnetic recording properties of nickel-copper alloys by performing an atomistic simulation of candidate mixtures using only first principles of quantum physics.

At the Supercomputing '95 conference, where it was demonstrated in these two applications, CUMULVS won the award for best interface and fault tolerance in the High Performance Computing Challenge. The CUMULVS program is also likely to win over many scientists.

The development of CUMULVS was supported by DOE's Mathematical, Information, and Computational Sciences Division and by DOE's Office of Energy Research, Basic Energy Sciences.

Computer Procedure Forgives Errors, Detects Proteins

Genetic information that determines who we are, what we look like, and how we function is encoded in the sequence of four different chemical bases forming steps of the twisted ladder of deoxyribonucleic acid (DNA). The traditional procedure for DNA sequencing for the Human Genome Project—gel electrophoresis—is highly efficient, but its error rate can be high. Errors in sequence introduce bases that are not really there or skip bases that are.

These errors make it difficult to identify proteins, which are made of various combinations of amino acids. Each of the 20 amino acids is coded for by a particular group of three bases. So, a sugar-digesting enzyme that contains 300 amino acids is a product of 900 bases. The base sequence, or nucleic acid alphabet, spells out the protein's amino-acid sequence, or protein sequence.

An ORNL algorithm accurately identifies proteins from erroneous DNA sequences.

If a base is erroneously missing in the sequence, the groups of three bases coding for each amino acid will fall out of sequence—a frame shift. Multiple frame shifts could prevent identification of a protein by its sequence. Repeating the sequencing 10 times allows accurate identification, but it's expensive.

To cut costs, ORNL has developed a frame-shift-tolerant protein sequence comparison algorithm that accurately detects proteins from a one-time DNA sequence. This step-by-step computerized procedure compares the experimental sequence with sequences in a database, considers all possibilities for errors, and finds the best match. In this way, proteins can be identified from corrupted sequences and errors can be determined.

The algorithm is part of the recently released Version 1.3 of the Gene Recognition and Analysis Internet Link (GRAIL) system, which is used by more than 1000 biomedical laboratories and biotechnology firms. The ORNL-developed GRAIL, which uses statistical analysis to separate meaningful words from genetic gibberish, finds genes in sequences through pattern recognition and through database comparisons for which the new algorithm is used. Recently, GRAIL pinpointed a gene responsible for a genetic disorder that can lead to paralysis, muteness, and death in boys—a theme of the movie *Lorenzo's Oil.*

Funding for this research has come from DOE's Office of Health and Environmental Research.

Crunching Numbers To Solve Difficult Industrial Problems

For some industrial firms, a new or improved product or process is not possible without solving complex problems. Sometimes these solutions can be obtained only by writing computer codes that run on parallel computers built from many nodes. To enter the esoteric world of codes, nodes, and other aspects of high-performance computing, industrial firms often require the help of appropriate computer experts.

Providing support and assistance to U.S. industry to smooth its path into high-performance computing is a prime expectation of ORNL's CCS. To help meet this goal, the CCS launched the Computational Center for Industrial Innovation (CCII). This DOE national user facility established in August 1994 hosts ORNL-industry collaborations in projects featuring high-performance computing. Thanks to our computational capabilities, CCII users are solving challenging, industrially relevant problems—problems that have previously eluded solution because of insufficient computational power or inadequate software availability.

A number of user agreements have been signed with a variety of businesses, software vendors, and other federal agencies. Consider these two examples of collaborations that illustrate CCII's impact.

Advanced military aircraft are being designed to take off and land quickly without the need for long runways. To explore aerodynamic properties of generic "advanced short takeoff and vertical landing" fighter aircraft, Lockheed Martin Skunk Works' scientists are using CCII facilities. Large, complex, three-dimensional models of this type of aircraft are simulated using sophisticated computational fluid dynamics codes. Shortened takeoff distances and vertical landings for these advanced fighters are made possible by using

The Intel Paragon is being used by industrial researchers to model advanced military aircraft and aluminum production processes.

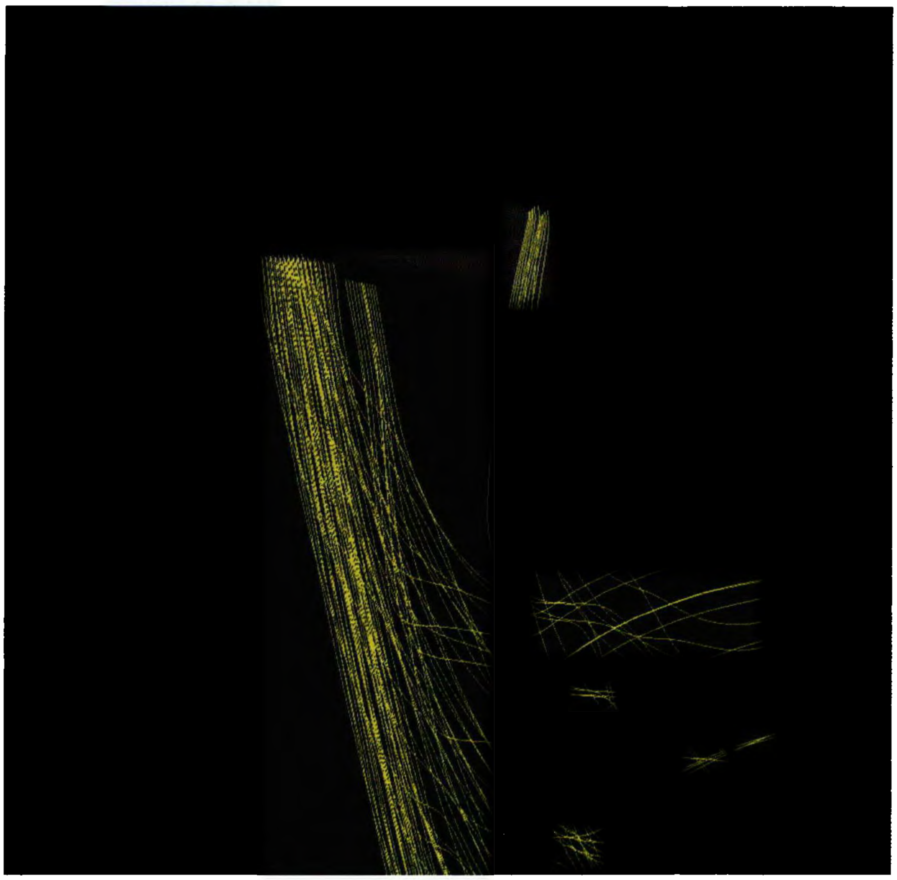


Image of an advanced short takeoff and vertical landing fighter aircraft simulated by Lockheed Martin Skunk Works' scientists using computers available at the Computational Center for Industrial Innovation at ORNL. The yellow beads are particle traces of the exhaust from thruster jets during a simulated takeoff.

small jet outlets under the aircraft's fuselage and wings to provide a large vertical thrust. Investigating a range of aircraft options using conventional experimental techniques is difficult and expensive. By using the high-performance computational facilities of CCS, Skunk Works' scientists can rapidly and accurately simulate many aircraft systems and flight strategies while reducing the number of costly physical experiments that must be performed.

Reynolds Metals' scientists are using CCII facilities to model industrial magnetohydrodynamic processes in which a magnetic field interacts with a conducting fluid. These processes are widely used in the aluminum industry for stirring, confinement, and control of liquid metal before and during casting operations. In addition, after the aluminum solidifies, inductive heating devices are frequently used both in the rolling of the aluminum ingots into strips and in the final heat treatment of the strips. Accurate modeling of these processes is important both for control of the existing manufacturing processes and design of future enabling technologies. This modeling, however, is computationally intensive because of the strong coupling among the various physical phenomena—heat transfer, electromagnetism, and fluid flow. Differences in magnitude between the size of the processes (typically meters) and the scale of change of the parameters that must be modeled (often millimeters) further complicate the calculations. Preliminary modeling of these complex industrial processes has been achieved by using the powerful Intel Paragon computers in the CCS.

Other projects under way at CCII involve automobile safety, materials processing and design, engineering design, nuclear reactor modeling, and manufacturing strategies. Additional companies are joining the center and many others, upon learning of CCII capabilities and accomplishments, are considering membership. By calling upon the capabilities and systems provided by the CCS to help open doors to industry, CCII is meeting an important U.S. need.

Computer Library Puts ORNL in Record Books

Imagine a special think tank in which hundreds of mathematical geniuses rapidly perform calculations all day long. Each mathematician has a brilliant personal assistant and a unique collection of notebooks, textbooks, and reference books in a cubicle. All the books make up the shared, or distributed, memory of the think tank. All personal assistants know the locations of all books in the think tank and the information in them. So, when Dr. Smith asks his personal assistant for special data, the assistant fetches the information by "borrowing" books from Dr. Jones and Dr. Miller and copying the appropriate pages for Dr. Smith.

At ORNL's CCS, the hundreds of parallel processors that make up the Intel Paragon XP/S 150 are like the think tank's mathematicians, except they work all night, too, and together can perform 150 billion calculations per second. Also, each processor has access to a clone of one brilliant assistant, whose job is to retrieve needed data from the shared memory; this shared assistant is the ORNL-developed Distributed Object Library (DOLIB). Such a collection of programs and routines available on each processor has enabled the Paragon to break a record.

A growing number of university and national laboratory researchers are interested in computer modeling of molecular dynamics. Their goal: to discover the physical behavior and properties of a system of molecules in motion in response to various forces. Until very recently, the largest molecular dynamics simulation ever undertaken involved six hundred million atoms. Using DOLIB, a team of researchers from ORNL and the state of New York shattered that record by simulating a system of 1 billion atoms of argon, calculating the forces involved as the gas atoms naturally approach and repel each other in a box.

DOLIB has also helped researchers using the Paragon predict the flow and fate of contaminant particles in groundwater, as well as changes in water balance in future climates under global warming scenarios. For these two problems, processors needed access to the shared memory, which contains all available information on horizontal flow (advection) of particles in groundwater or moisture in air.

The DOLIB team also surmounted another obstacle: the unacceptably long times required to receive data from the mass storage disk and get calculated results from the computer during a computation. To solve this input/output (I/O) problem, the team developed the Distributed Object Network I/O Library (DONIO), which makes use of DOLIB. DOLIB finds the processors that have the needed data in memory, and DONIO makes copies at high speed of the portion of the mass storage disk holding the data (as much as 100 gigabytes).

In an acoustic-wave propagation application of interest to the oil industry, DONIO reduced I/O time from more than 9000 seconds to 273 seconds (a reduction of 97%) and in a molecular dynamics application, from 1200 seconds to 50 seconds (a reduction of 96%). Now, the time it takes to move the data in and the results out is almost as short as the brief time required to do the actual calculations. When it comes to minding the storage, ORNL soon may be breaking other records.

Our DOLIB programs have enabled our supercomputer to break a record in molecular dynamics modeling.

Computing Future: Fast Machines on Fast Networks

The building blocks of a lightning-fast parallel supercomputer are small computers linked together that simultaneously solve pieces of a complex problem. So most computing

By linking ORNL and Sandia supercomputers via a high-speed network, a virtual computer will be created to solve nearly impossible problems.

experts agree that the next logical step in high-performance computing is to link two of these fast parallel supercomputers together. But what if two of the world's fastest computers are separated by hundreds of miles? Then the challenge becomes finding a way to connect them through a very-high-speed network to create one of the world's largest virtual computers.

ORNL scientists and colleagues from the CCS and Sandia National Laboratories (SNL) are preparing to demonstrate the effectiveness of such an arrangement. These two laboratories possess a striking level of computing power, making such a demonstration noteworthy.

The basic idea is to link the two largest Intel Paragons (an 1840-processor XP/S 140 at SNL and a 2048-processor XP/S 150 in the CCS) over a high-speed Asynchronous Transfer Mode (ATM) network to solve problems too large for either machine alone—extraordinarily formidable problems relevant to both ORNL and SNL. By extending computational parallelism into the network and surmounting technical hurdles on the path to virtual high-speed computing, the researchers will advance the technology.

To use this distributed computing power effectively requires codes developed with the ORNL-SNL communication time in mind. One such code is a materials science code written by ORNL researchers to model the magnetic structure of complex magnetic alloys. Another is a global change code that couples the atmosphere (code prepared at ORNL) and the ocean (code prepared at Los Alamos National Laboratory) to provide a superior climate simulation over extended times. Additional codes that address the safety of defense weapons are being prepared.

To enable the two Paragon computers to work together, ATM boards were specially designed and built for them by the small company, GigaNet, with support from SNL. The excellence of these boards was demonstrated through high-performance links connecting the SNL, ORNL, and Intel booths at the Supercomputing '95 exhibition in San Diego.

Our work is focused on ensuring compatibility among codes, operating systems, ATM, and parallel virtual machine software and addressing performance issues so that scientific goals can be met. Significant questions concerning network connections and network availability are being addressed. The support of the Energy Sciences Network (ESNet), DOE's branch of the Internet, continues to be important. Given the significance of scientific problems that can be solved only by high-performance systems linked by a high-speed network, anticipation for a functioning virtual supercomputer is high.

Virtual Labs Soon Will Be Reality

Can scientists scattered all over the United States do collaborative research

Scientists elsewhere may soon remotely operate research equipment at ORNL facilities.

Mona Yethiraj, an ORNL scientist, checks a small-angle neutron scattering spectrometer that will be operated remotely for neutron science experiments at ORNL's High Flux Isotope Reactor.

at ORNL using neutron scattering? ORNL hopes to show soon that an experiment can be performed at one of its user facilities—from a distance.

Researchers working throughout the United States might do better science if they collaborated with their colleagues rather than competed against them. More effective collaborations could eliminate duplication of effort while improving the quality of research results and technology developments.

The high cost of travel and organizational roadblocks often prevent many potentially valuable collaborations. However, these barriers can be eliminated through use of computing and communication technologies that permit remote operation of research equipment, bringing user facilities to users "over the network." Such virtual laboratories, or "collaboratories" that transcend physical distance and organizational structure, are one goal of the DOE 2000 program.

Emerging from the DOE Offices of Defense Programs and Energy Research, the program's goal is to provide tools and systems, software and hardware, to make possible highly effective collaborative research projects involving geographically dispersed scientists and facilities. What are the benefits? Reduced travel costs. Improved quality and efficiency of research. A new opportunity to exploit DOE strengths in high-performance computing and communication. A way to maximize collective use of DOE national user facilities and other resources by appropriate researchers at each site and from far away.

ORNL and other DOE national laboratories are implementing the DOE 2000 program by establishing a remotely accessible environment through video links, cameras, interactive laboratory notebooks, and software to control instruments, adjust samples, and view and manipulate data from home pages of the Internet's World Wide Web. Two ORNL user facility instruments have been put on line for remote operation. They are the HF 2000 cold field-emission transmission electron microscope at the High Temperature Materials Laboratory and a small-angle neutron scattering spectrometer at the High Flux Isotope Reactor (HFIR). By late 1996 we hope to have widely scattered non-ORNL users examining the structure of specimens and doing neutron scattering experiments over the network. We hope they find collaborative research from a distance as pleasant, effective, and collegial as that on site.

ORNL has helped develop an advanced system to rapidly retain and access digital information.

High-Performance Storage System for Fast Computers

As computers become faster at a remarkable rate, there is a corresponding surge in the amount and availability of electronic information. For the CCS, the quantity of digital information that must be retained, properly characterized and catalogued, and readily accessed—all with absolute accuracy—is already enormous. And the rate of growth is phenomenal.

To deal properly with the onslaught of information, the CCS in collaboration with the DOE Atmospheric Radiation Measurement Project has assembled a storage environment with a capacity of about 100 terabytes (tera means trillion, or a million million). The software that coordinates and structures the data within this hierarchical disk-and-tape storage system is currently NSL-Unitree. However, this serial software will be far too slow in the near future.

Recognizing the impending demands on storage software some years ago, a consortium from ORNL, Lawrence Livermore National Laboratory, Los Alamos National Laboratory, Sandia National Laboratories, and IBM Government Systems designed and initiated the development of the High-Performance Storage System (HPSS). Its purpose is to address the storage access and management needs of very large, high-performance computing and data management environments. It is designed to move large data files between storage devices and parallel or clustered computers faster, more efficiently, and more reliably than today's commercial storage system software products. To accomplish this goal, HPSS uses a network-centered architecture and parallel transfers with target data rates reaching many gigabytes per second.

The ORNL-CCS team working on HPSS was responsible for developing strategies and systems for the entire storage environment. Initial tests of HPSS within the CCS system will begin soon. The capabilities of HPSS for parallel transfers will be of particular value in the CCS because of the 14 tape drives in our storage environment.

A number of major computational centers are implementing HPSS; all of the development laboratories have plans to do so. Sandia National Laboratories is using HPSS for storage with its Intel Paragon. We anticipate that HPSS will become the de facto storage system software standard for high-performance computers.

The work is supported by DOE, Defense Programs Office, Accelerated Strategic Computing Initiative.

DOE Award for GMR Research

Using parallel computers in ORNL's CCS, scientists better understand a physical effect that already has magnetic appeal: it allows more data to be packed on computer disks. These insights into the giant magnetoresistance (GMR) effect have earned three ORNL researchers the prestigious DOE-Basic Energy Sciences Division of Materials Sciences Award for Outstanding

Scientific Accomplishment in Metallurgy and Ceramics for 1995.

Discovered in France in 1988, GMR is a large change in a magnetic material's resistance to the flow of electrical current, caused by an applied magnetic field. It was found then that electrical resistivity of a layered iron-chromium film was lowered when the material was placed in a magnetic field. This effect allows GMR "read sensors" to read data crammed into high-density disks as tiny regions of magnetization.

By working at the atomic level, performing first-principle calculations of variations of electrical resistivity in metal alloys, we hope to improve magnetic storage systems. We are now working with IBM on the use of GMR to make higher-density disk drives.

In our computer modeling of the GMR effect in materials that have structures "layered" at the atomic scale, we found that electrical resistivity drops when the directions of two layers' magnetisms are aligned by an external magnetic field. We used parallel computers to calculate conductivity (the inverse of resistivity) and to calculate the magnetic field strengths required to align fields in magnetic layers in systems in which copper layers are embedded in cobalt.

Our calculations showed a waveguide effect for electrons in the cobalt-copper system. Like light waves moving a long distance in an optical fiber for telecommunications, some electrons travel far in copper without being scattered because they are trapped in the copper, which has lower resistivity than cobalt.

Comparison of our calculations with IBM's measurements implied that, if smoother interfaces could be made between alternating layers of cobalt and copper, exciting developments could follow. Examples might be computer operating memory that is immune to power disruptions and ionizing radiation and GMR motion sensors that increase the efficiency and safety of our home appliances, automobiles, and factories. Future magnetoelectronic devices could be attractive.

The research was sponsored by DOE's Office of Defense Programs, Technology Management Group, through a cooperative research and development agreement with IBM and DOE's Office of Energy Research, Basic Energy Sciences.

We're working with IBM on use of the giant magnetoresistance effect to make higher-density disk drives.

ORNL's Bill Butler (front), Xiaoguang Zhang, and Don Nicholson received the DOE–Basic Energy Sciences Division of Materials Sciences Award for Outstanding Scientific Accomplishment in Metallurgy and Ceramics for 1995. Much of their work was done using ORNL's Kendall Square Research parallel computer (in the background). *Photograph by John Smith.*

Computer Code Probes Mysteries of Magnetism

About 25 years ago, when Malcolm Stocks began working at ORNL as a postdoctoral scientist, he was puzzled by some new neutron scattering results obtained by Joe Cable (now retired).

The results offered fresh insights into the magnetism of a copper-nickel alloy—a simple, well-studied metallic alloy made up of copper and nickel atoms almost randomly distributed on an underlying crystal (face-centered cubic) lattice. Nickel is a ferromagnetic element, and copper is nonmagnetic. If copper is added to nickel, the alloy becomes less magnetic, losing its magnetism when it's 50% copper.

Over the next several years Stocks and others developed sophisticated methods for calculating electronic properties of disordered alloys. While successful, calculations based on these methods described the magnetism of copper-nickel alloys in terms of an "average" magnetism (magnetic moment) associated with nickel atoms, which decreased as copper was added to the alloy. But results from Cable's experiments at ORNL's HFIR suggested that nickel sites throughout the alloy sample had magnetisms ranging from high to low, depending on their environment. Cable's findings indicated that a nickel site's magnetism is much higher if it has nickel atoms nearby and much lower if it has copper neighbors.

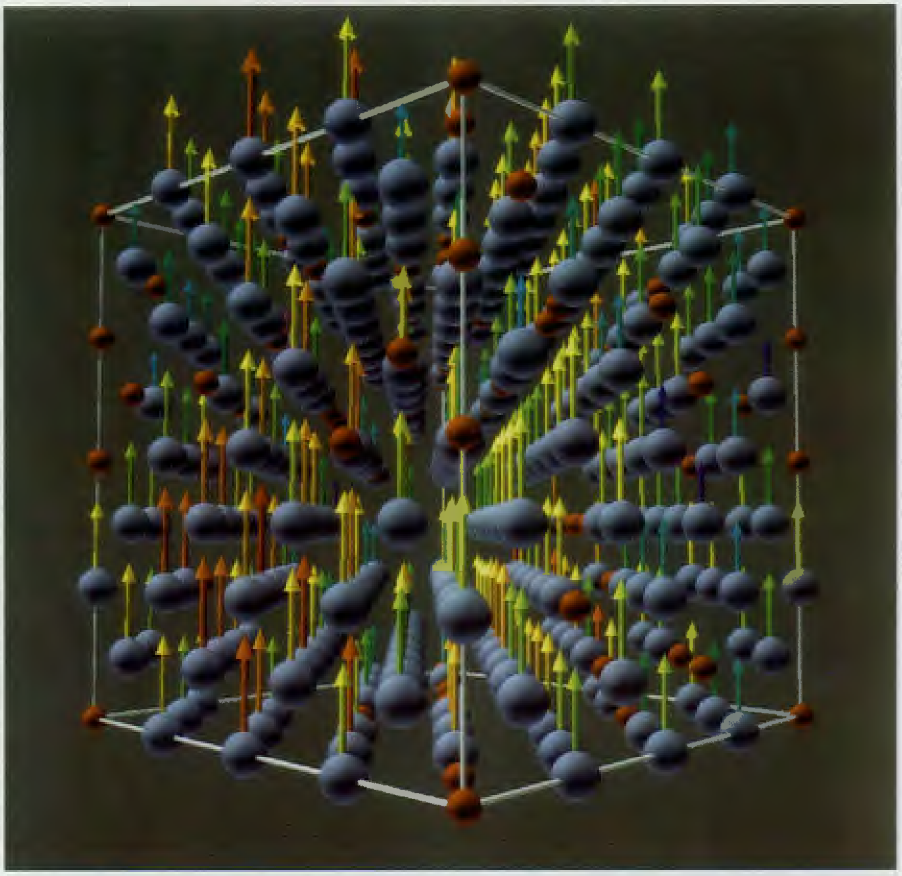
These curious results stuck with Stocks for years. In the 1990s, when the Intel Paragon supercomputer was being installed, he saw an opportunity to use it to model alloy magnetism at a more detailed level and simulate the neutron scattering experiment directly. But first he and his colleagues had to develop a completely new type of computer code that could perform first-principle calculations on hundreds to thousands of atoms. In this study they carried out first-principles calculations on 256 copper and nickel atoms randomly distributed in a box to simulate the disordered alloy. The calculations were performed on 256 parallel-processing nodes of the Intel supercomputer.

Stocks was amazed and pleased to learn that the Paragon's calculations strongly support Cable's results. The calculation not only gave excellent agreement with the measured neutron-scattering cross sections but also provided an atom-by-atom picture of magnetism. From this it can be seen that the magnetic moments are higher for nickel sites whose neighbors are nickel atoms having strong magnetism than for nickel sites surrounded by (1) nickel atoms having weak magnetism or (2) virtually nonmagnetic copper atoms.

The winning combination of code and computer is now being applied to more mysteries of magnetism, such as why and how ferromagnetic materials lose their magnetism at specific temperatures and whether the direction of atomic-level magnetic moments in alloys and magnetic multilayers can vary in previously unsuspected ways. Results from our investigations using nodes and neutrons could help improve the design of alloys to give them better magnetic properties for data storage and power generation.

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

Calculations by a new supercomputer code confirm neutron data on magnetism in a copper-nickel alloy.



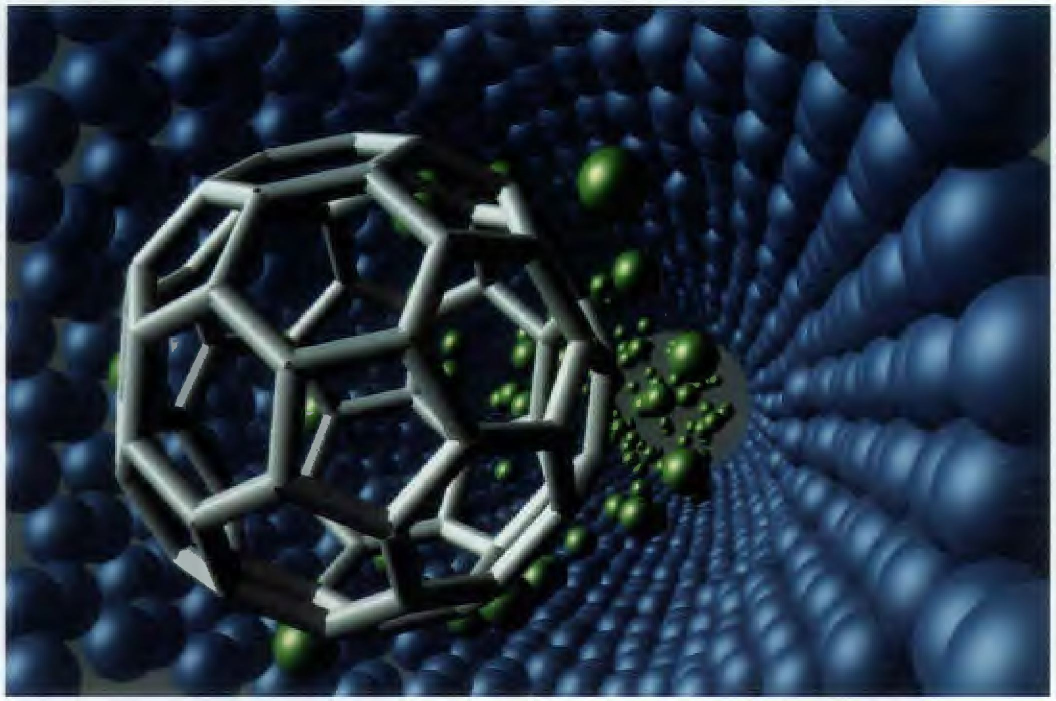
Magnetisms of individual atoms in a copper-nickel alloy are calculated using a new computational method and ORNL's massively parallel Intel Paragon supercomputer.

Explaining How Solids Melt

Chocolate melts in our mouths, but exactly how it turns from solid to liquid isn't clear in our minds. We don't really understand precisely how ice melts as it cools our drinks. Some of the world's top scientists have tried—and failed—to explain melting at the atomic level.

Recently, three ORNL researchers have used the Intel Paragon XP/S 35 to help confirm a theory developed in the 1970s about how substances melt in two dimensions. Using an interatomic force model often used for rare-gas

We have developed computational tools to do reality checks on designs for nano-scale devices.



In this holographic representation of a computational simulation of a nano-device the size of a dust mote, the tube is formed from carbon atoms (blue tennis balls), the soccer ball is a buckyball, and the green squash balls are flowing helium atoms that penetrate and push the buckyball "piston" through the tube (see cover.)

solids, they simulated two-dimensional systems containing 576, 4,096, 16,384, 36,864, or 102,400 atoms.

Results for the two largest systems show the existence of a new "hexatic" phase between the solid and liquid phases, as predicted by the theory. This two-dimensional simulation helps explain the melting process. It also may help researchers gain an understanding of how substances melt in the real world—in three dimensions.

The research was supported by ORNL's Laboratory Directed Research and Development Program.

Computational Checks on "Nanomachines"

When you hold ORNL's plastic card for guests to the light—the Kodamotion card made by Kodak—you see what looks like a soccer ball and a few green squash balls rolling in a tube made up of blue tennis balls glued together. In this holographic representation of a computational simulation of a nanodevice (from nanometer, a billionth of a meter), the tube is formed from carbon atoms, the soccer ball is a buckyball, and the green balls are flowing helium atoms that can penetrate and push the buckyball "piston" through the tube. By turning the Kodamotion card slowly, you see interactions among all the atoms, even the naturally vibrating "balls" in the graphite tube.

Nanotechnology futurists dream of microbe-sized machines built from a few million atoms. They envision robots the size of a dust mote that manufacture therapeutic drugs or swim along eating stream pollutants or slaying cancer cells in the bloodstream. They envision "smart" materials embedded with nanosensors that alert operators to atomic-level defects, providing adequate time to repair or replace equipment before it can fail. Already on the scene are "optical tweezers"—laser beams that spin microscopic rotors in liquid and can be used to dissect bacteria and manipulate molecules at room temperature.

But will the dreamers' designs work as intended? Will the devices be stable? What are their operational limits? Our chemical physicists have developed tools to do reality checks on these ideas. They have adapted algorithms to solve molecular dynamics equations quickly on parallel computers—in a minute for every hour previously required. Now, computational simulations of the mechanical properties of molecular bearings and gears are feasible. Interactions of a gas, liquid, or laser light with a nanomachine part can be precisely modeled.

Computational simulations can lead to new discoveries. ORNL's simulation of a design for a nano-scale "frictionless" bearing revealed the new phenomenon of atomic-scale friction, suggesting that a redesign is needed to reduce this effect.

Our chemical physicists are now working under a CRADA with Angstrom Tools, LLC, to develop user-friendly software to design and test proposed nanostructures and devices. They are convinced that practical nanomachines are in the cards.

The research has been supported by a grant from ORNL's Laboratory Directed Research and Development Fund and by DOE's Office of Energy Research, Basic Energy Sciences, Materials Sciences Division. **ornl**

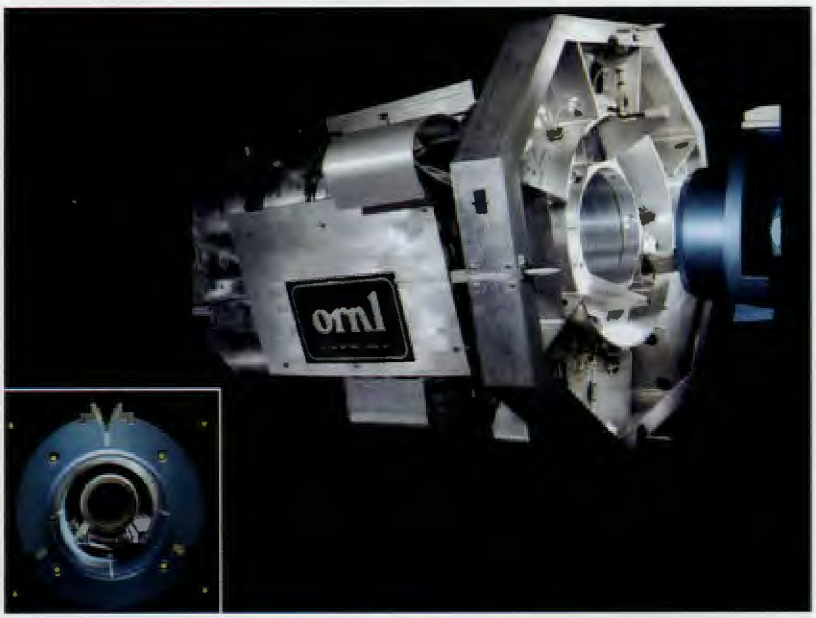
Robotics Technologies Devised for Defense, Decontamination

Picture a battlefield in the late 20th century. Without armored protection, soldiers in a truck locate ammunition, prepare it for firing, hop out, and manually reload a howitzer—a cannon mounted on a tracked vehicle that fires shells with a medium velocity and high trajectory. They look around nervously, hoping they don't get hit by an enemy projectile.

Now, picture a battlefield in the early 21st century. A self-propelled howitzer and a companion ammunition resupply vehicle roll across the ground. A robotic arm that "sees" through computer vision technologies delivers it to the howitzer. No soldiers are in sight; they are hidden inside the armored vehicle. Rearming weapons systems has become safer and more efficient.

This 21st-century robotics technology has already arrived and is maturing at ORNL. On November 28, 1995, ORNL demonstrated an automated ammunition processing, handling, and delivery system for a project manager of the U.S. Army. Called the Crusader system, it combines a self-propelled howitzer and a vehicle to rearm it. The Army plans to field this weapons system in 2005.

We developed technologies for the Army to automatically and safely reload cannons.



To automatically rearm a cannon, the end section of the robotic arm approaches docking with a howitzer port. The inset shows the port's sensors that make a pattern for the arm's "eyes" to see and recognize as the docking point. On the battlefield infrared sensors will enable docking without detection by the enemy. *Photograph by Tom Cerniglio.*

ORNL has developed several technologies for the Crusader system. They are

- a six-degree-of-freedom, articulated robotic transfer arm that can be either manually controlled or automatically docked with the howitzer;
- an automated ammunition processing center that removes the lifting eye (portable part of the round of ammunition), inserts a fuze, weighs each projectile, and marks it in preparation for firing; and
- an automated ammunition recognition system that keeps track of ammunition loaded into and fired from the howitzer.

The technologies have met Crusader System requirements for increased efficiency in operation and armored protection for soldiers during the automated rearm process. Demonstration of the Crusader system technologies was the culmination of a three-year, $15-million collaborative effort of engineers, computer specialists, and technicians from eight ORNL divisions.

Besides defense, we are devising robotics technologies for the decontamination and dismantlement of reactors and other radioactive equipment. On September 19, 1995, our robotic and remote-handling systems developed for this purpose were demonstrated for DOE.

When remotely operated machines are needed to do work too hazardous for humans, ORNL is an important part of the picture.

Funding for this work was provided by the U.S. Army and DOE's Office of Environmental Management.

Science Education: Teaching Materials

One of the first lessons we learned in kindergarten was to share. ORNL researchers have often shared their knowledge of how to "do science" in a laboratory setting or in the field. All we need is an interested audience. Because DOE seeks to improve science education and encourage students of all ages to specialize in science and engineering, a large fraction of our audience includes students and faculty from elementary and secondary schools, colleges, and universities. Some of them help conduct experiments in the labs, getting hands-on experiences; others are eagerly learning in classrooms, often with their hands up. For everybody it's usually an interactive experience, because many teachers and students do real work and provide fresh ideas—they give something back to the Lab.

Materials Science Alliance. Thanks to an educational and research collaboration begun in 1995, minorities will have a greater chance to explore materials. In October, a new Materials Science Alliance was planned as a partnership involving ORNL's Solid State Division, five materials-related DOE user facilities at ORNL, and historically black colleges and universities and other minority educational institutions throughout the southeastern United States. About 100 academic and governmental participants attended the planning meetings in Oak Ridge, which were supported by DOE's Division of Materials Sciences. In 1995 the Solid State Division managed a collaborative research program with Alabama A&M University in which eight students participated in ion implantation research at the Surface Modification and Characterization Collaborative Research Center.

Teacher Leadership Institute. Teachers in junior and senior high schools can reinforce their knowledge of science by doing experiments in the laboratory or field. Such exercises could strengthen their teaching skills. So could knowledge of innovative strategies for transmitting science concepts to students and better ways to evaluate whether the messages are received and understood—and to follow up if they are not.

During the summer of 1995, ORNL's Office of Science Education established a three-year, secondary-level Teacher Leadership Institute. It is supported by the 13-state Appalachian Regional Commission, which since 1991 also has sponsored an on-site Summer Science Honors Academy, conducted in cooperation with ORNL's Metals and Ceramics Division. In the three-week residential program in Oak Ridge, small teams of teachers participate in "research immersions" in five ORNL divisions to improve their knowledge of science content. In one example, a high school teacher worked with a researcher to produce an educational demonstration video on high-temperature superconductivity. The teachers also go to class to learn leadership skills to help them better share their science knowledge with their students.

Minority students are exploring materials, and teachers are learning leadership skills.

Eric Williams (left) and Melvin Spurlock, graduate students at Alabama A&M University, help perform materials research at ORNL's Surface Modification and Characterization Research Center. Here, Spurlock examines a sample in a target chamber, which will be implanted by ions from an accelerator.

Development and Operation of National Research Facilities

ORNL is the home of 16 sophisticated experimental science facilities that are available to users nationwide and, in most cases, throughout the world. Twelve are officially designated by the DOE as "user facilities." Two new user facilities established in 1995 (and described in this section) are the Metrology Research and Development Laboratories and the Metals-Processing Laboratory User Center (MPLUS).

These research facilities serve scientists and engineers from universities, industries, and other government laboratories, as well as ORNL staff. They simultaneously contribute to DOE missions and other national science and technology goals by minimizing unnecessary duplication of effort, promoting beneficial scientific interactions, and making the most effective use of costly and, in many cases, unique equipment.

The development and operation of these facilities require the broad interdisciplinary human and technical resources available at ORNL. These facilities are supported by specific elements of the research infrastructure ranging from atomic physics to genetics. They rely on operational expertise in diverse arenas such as research reactors, particle accelerators, bioprocessors, and extensive environmental research reserves. At various stages of a facility's lifetime, we provide expertise in design, engineering, project management, computing-data acquisition, and instrumentation, as well as resources to support user services and an administrative infrastructure.

Our facilities support DOE missions in basic energy sciences, nuclear physics, advanced materials development, biotechnology, genetics, environmental science and technology, and energy efficiency. The facilities offer a strong educational benefit; many graduate students use them in their thesis research, and interactions are increasing with school teachers and K-12 students. The facilities also provide direct support to help our many industrial users become more competitive.

Besides the two new ones, ORNL user facilities and centers include the Atomic Physics EN Tandem Accelerator, Bioprocessing Research Facility, Buildings Technology Center, High Temperature Materials Laboratory, Holifield Radioactive Ion Beam Facility, National Environmental Research Park, Neutron Scattering Research Facilities, Oak Ridge Electron Linear Accelerator, Shared Research Equipment, Surface Modification and Characterization Research Center, High Flux Isotope Reactor, Center for Computational Sciences, and Mammalian Genetics Facility (including the Mouse House).

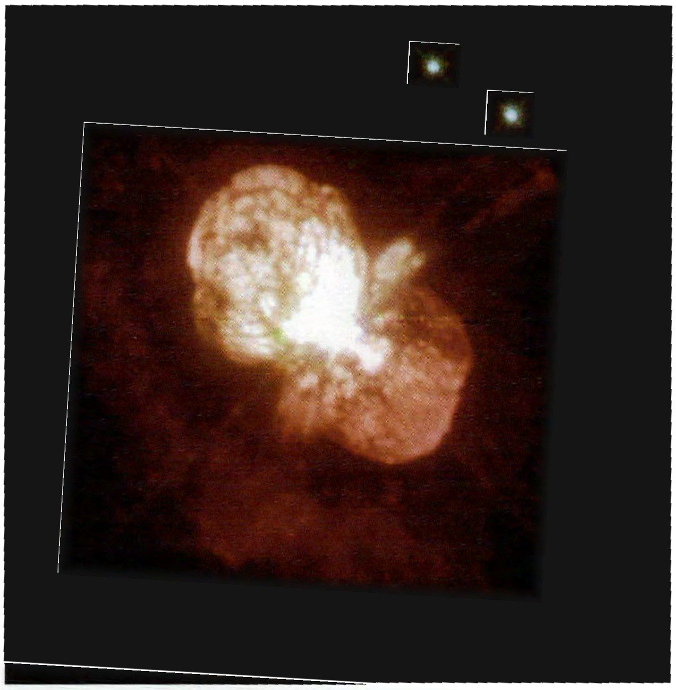
Holifield Radioactive Ion Beam Facility: User Center Will Reach for the Stars

HRIBF's radioactive ion beams will be used for nuclear structure and nuclear astrophysics research.

The orbiting Hubble Space Telescope and Compton Gamma Ray Observatory satellites constantly beam down information from the stars. Soon researchers at the Holifield Radioactive Ion Beam Facility (HRIBF) will shed even more light on the life and death of stars by conducting down-to-earth experiments. HRIBF, which should be ready for its first experiments in October 1996, is the only U.S. facility dedicated to producing and accelerating intense beams of radioactive nuclei that occur naturally only in outer space.

Recently, the Compton Gamma Ray Observatory detected radioactive aluminum-26 in the cosmos. How? It measured the energies of gamma rays characteristic of the decay of aluminum-26. HRIBF researchers, using an ORNL cyclotron and the world's largest electrostatic accelerator, will be able to make measurements to understand how such elements are produced. For example, already physicists have determined the rate at which aluminum-26 is produced and the energy released in its formation by bombarding a stable magnesium-26 target with protons to make the radioactive isotope aluminum-26. Such information is of interest because heavier elements such as aluminum are formed in nova and supernova. However, in these spectacular stellar explosions many of the reactions involve nuclei that do not occur naturally on the earth, which has become increasingly stable over the past 5 billion years. Therefore, accelerated beams of radioactive nuclei are needed to provide data to understand many nuclear processes during stellar explosions. Such measurements using radioactive ions will be the forte of the HRIBF.

Element synthesis and energy generation during stellar explosions depend crucially on rates of thermonuclear fusion reactions in which radioactive nuclei are formed as isotopes capture protons; one such important reaction is the capture of protons by fluorine-17 nuclei to produce neon-18. However, because the relevant nuclei are radioactive, direct measurements of these reaction rates have not been possible at existing accelerators. For example, it is not known whether nova explosions produce only low-mass nuclei (up to fluorine) or also nuclei up to iron and beyond. Direct measurements of the rates of such crucial fusion reactions will help to resolve these discrepancies. The HRIBF will provide this important information.



The remnants of Eta Carina as seen through the eyes of the Hubble Space Telescope. Such spectacular stellar explosions produced many elements and dispersed them to the cosmos. In the 1840s, this nova briefly was the second brightest star in the sky.

About one-third of the HRIBF's work will be devoted to nuclear astrophysics using beams of, for example, radioactive fluorine, chlorine, and sulfur. One question that may be tackled is this: How are light elements up to iron synthesized through rapid hydrogen burning processes in binary star systems? In this process, a white dwarf, made of mostly heavy elements, pulls hydrogen away from an expanding red giant, resulting in a thermonuclear explosion that shoots jets of proton-rich heavy elements into outer space. Such processes are thought to be the largest thermonuclear explosions in the universe.

Two-thirds of the research at HRIBF will be concerned with nuclear structure. Nuclear structure studies will include searches for short-lived deformed nuclei shaped like footballs, pears, cigars, and perhaps even bananas! These nuclei will be formed when a radioactive beam strikes a target. Heavy radioactive nuclei having nearly equal numbers of protons and neutrons (such as tin-100, a "holy grail" isotope) will be extra stable, enabling physicists to better understand the effects on nuclear structure of variations in neutron and proton numbers, as well as the limits of stability. Other nuclei will be quite unstable, enabling physicists to observe a new form of radioactivity—emissions of protons.

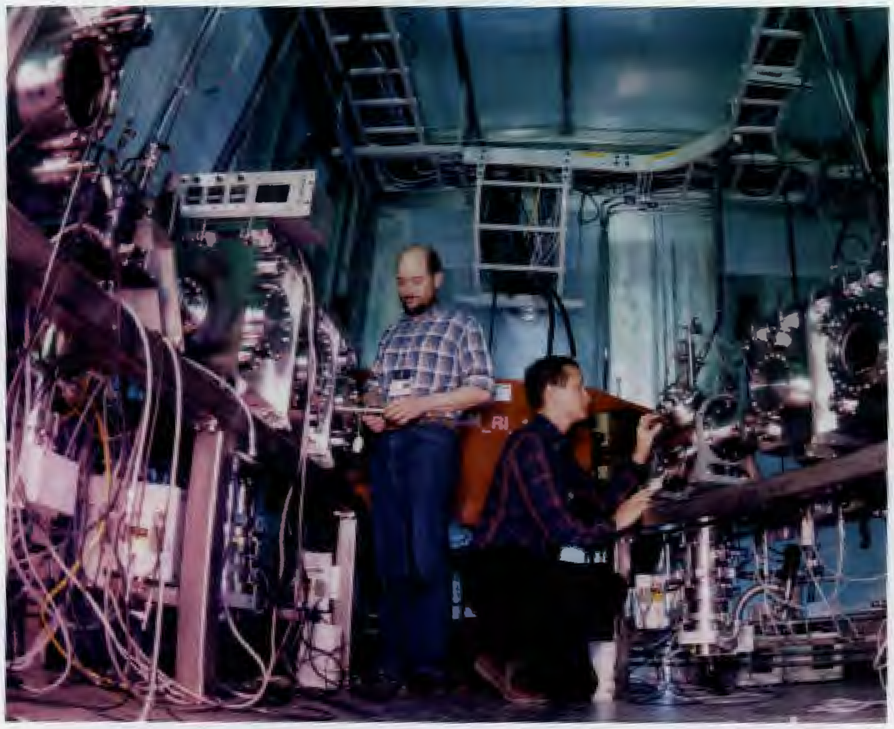
Carl Gross (left) and Chang Hong Yu inspect a recoil mass spectrometer that will help them decipher nuclear structure at ORNL's Holifield Radioactive Ion Beam Facility. ***Photograph by Tom Cerniglio.***

accelerated stable, heavy ions. If an energy boost was required, the Oak Ridge Isochronous Cyclotron (ORIC) provided it for ions exiting the accelerator. Now, the roles have been reversed. ORIC will slam an intense light-ion beam, such as protons or helium-3 nuclei, into a target. Collisions between projectile and target nuclei result in many radioactive products. After diffusing from the target, the desired isotope is magnetically separated from the other products. Atoms of this isotope are converted to negative ions, which are accelerated through the tandem as a radioactive ion beam. The accelerated radioactive ions will smash into a target, producing reaction products that can be measured in a variety of experimental stations at the HRIBF. Most of the radioactive beam experiments will probably use one of two new experimental stations, which are being constructed to select the very rare reactions of interest from the background of the beam and the products of less exotic reactions.

The astrophysics experiments will use the recently installed Daresbury Recoil Separator from England to measure the rates of fusion reactions between the incoming radioactive ions and hydrogen and helium targets. The nuclear structure experiments will use an even larger recoil mass separator together with a variety of detectors to detect and measure energies of gamma rays, protons, alpha particles, and eventually neutrons.

No materials science research program has been established yet for HRIBF, but physicists there are hoping such a program will be supported. One proposed experiment would aim to make a diamond transistor. A beam of radioactive carbon-11 could be used to implant radioactive carbon-11 ions in a diamond target. After irradiation the diamond could be heated. The carbon-11 atoms would anneal into the diamond lattice as carbon, but after some hours they would all decay to stable boron-11. Thus, a substrate of boron could be produced in the diamond crystal. It is expected that such a diamond transistor could operate at very high power.

By the end of 1995, the HRIBF was completed on time and within cost with the help of ORNL's skilled crafts personnel. Two accelerators in the heavily shielded facility had to be reconfigured. Originally, Holifield's 25-million-volt tandem accelerator



Paul Mueller (left) and Alan Tatum work on the 300-kilovolt Radioactive Ion Beam Injection Platform, where radioactive atoms are produced, ionized, and selected for injection into the 25-megavolt tandem accelerator. ***Photograph by Lynn Freeny.***

In preparing the facility for experiments, tests have been performed to estimate how fast and efficiently a stable arsenic beam can be extracted from a germanium target bombarded by protons. A newly installed robot also has been tested. After the target ion source assembly becomes radioactive and a new target is needed, the robot will pick it up, put it in a cask, and place the package on a conveyor belt to be carried away. Then the robot will place a new ion source on the insulated, high-voltage platform.

Thirty-four letters of intent have been received from 99 researchers at 36 institutions in 17 states and 6 foreign countries proposing experiments at the HRIBF. The HRIBF user organization consists of about 300 scientists from the United States and 20 foreign countries. Experiments with radioactive ion beams are expected to start in 1997. As we approach the third millenium, the world can expect research results from a unique facility that should be of stellar quality.

The facility is supported by DOE, Office of Energy Research, Office of High Energy and Nuclear Physics.

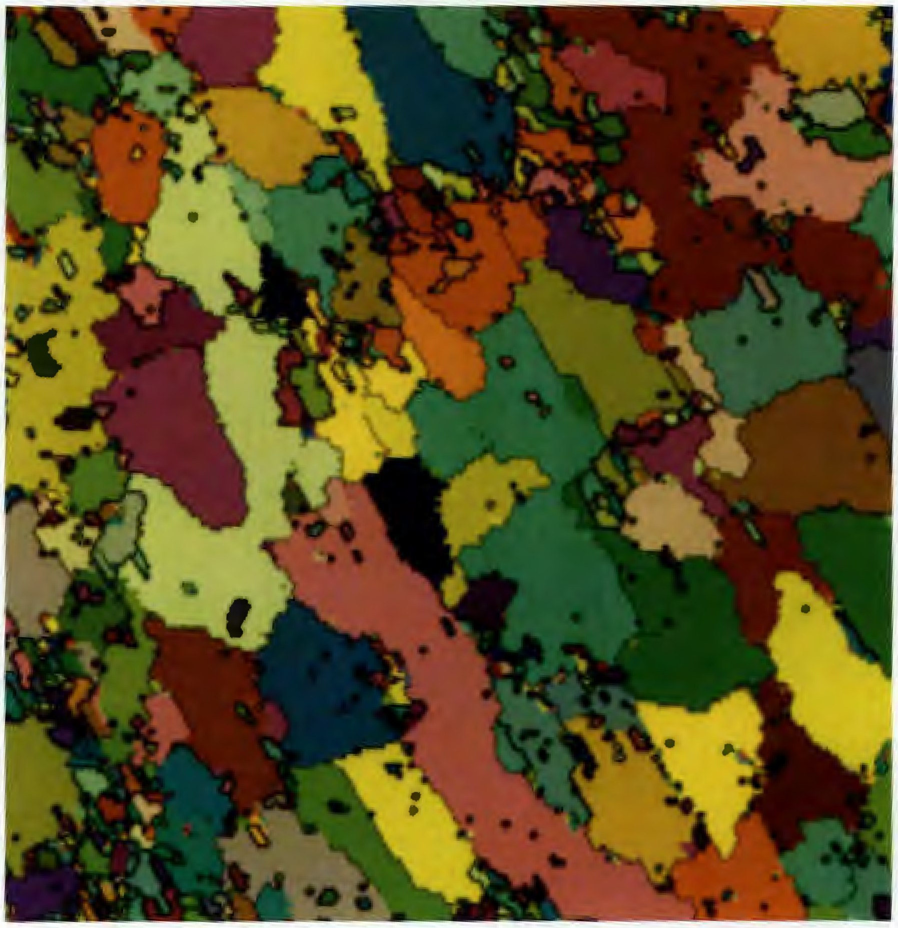
SHaRing Our Microscopy Expertise

ORNL has gained visibility for its work with tools to image the seemingly invisible. Its Shared Research Equipment (SHaRE) program is one of four DOE electron microscopy facilities for materials science studies to receive support through the Presidential Scientific Facilities Initiative (funded by DOE's Office of Energy Research, Basic Energy Sciences, Division of Materials Sciences); the other ORNL facilities to win support from this $100-million initiative are the High Flux Isotope Reactor and the HRIBF. Because of the boost in funding for the SHaRE program, the number of users of the facility should double previous annual counts.

To characterize the structure, chemistry, and mechanical responses of materials and solve materials science problems, ORNL and outside researchers have been sharing a variety of SHaRE tools: transmission electron microscopes, scanning electron microscopes, atom probe field ion microscopes, atomic force microscopes, and mechanical property microprobes. Use of these microanalytical techniques has enlarged the Laboratory's reputation in materials sciences.

We are a world leader in using atom probe field ion microscopy to do chemical analyses on samples with single-atom resolution. The three-dimensional atom probe concept developed at ORNL will provide the best and most rapid detection capabilities in the world. By imaging nickel aluminide alloys, we gain insights into how trace additions of boron and zirconium improve the alloy's properties. In the same way, we glean information on the role of copper-enriched precipitates in causing

Our Shared Research Equipment program played a key role in the development of superconducting wire.



This view of ORNL's rolling-assisted biaxial textured substrate (RABiTS) was provided by the SHaRE program's new field-emission-gun scanning electron microscope. Diffraction patterns formed by electrons backscattered off the sample reveal grain orientations. From these data, grain boundary misorientations were calculated and shown by color coding. Because grain boundary misorientations in the sample are mostly less than 10 degrees, superconducting properties are effectively preserved.

embrittlement in reactor pressure vessel steels and on the influence of neutron irradiation and thermal annealing on the steels' copper content.

A new field-emission-gun scanning electron microscope at the SHaRE facility has played a key role in the development of the foundation of a flexible superconducting wire that can carry considerable current (see the highlight on p. 40). The microscope maps texture (or grain orientation) by analyzing patterns of electrons backscattered from crystalline planes of atoms. Combined with other techniques available using the scanning electron microscope, this mapping capability can determine the relative orientation, composition, and surface topography of all crystalline grains in a solid sample and the location and interconnection of grain boundaries.

Using this instrument, we observed the relative grain orientations in some superconducting materials and compared them with measured variations in electrical conductivity in these samples. This information guided the development of a substrate, or textured template, with properly aligned grains for the base metal and overlying buffer layers. Our texture mapping showed that this substrate-buffer system forms a template on which atoms of the superconducting material deposit so as to form a continuous path for electrical current, increasing its current density. Because of the microscope's value to superconductor development, it was jointly supported by DOE's Office of Energy Research, Basic Energy Sciences, and DOE's Office of Energy Efficiency and Renewable Energy.

We know that little things mean a lot, and we SHaRE our tools and talents.

Funding for the project was provided jointly by DOE, Office of Energy Efficiency and Renewable Energy, Office of Utility Technologies and by DOE, Office of Energy Research, Division of Materials Sciences.

ORNL offers industry some of the world's best and most precise measurement instruments.

At the Metrology Research and Development Laboratories facility, mechanical engineer Ruth Anne Abston prepares a mass flow controller for testing by ORNL's prize-winning gravimetric calibrator, which measures gas flow rates. *Photograph by Curtis Boles.*

Metrology Lab Measures Up

You own a small company that needs precision measurement and testing equipment. But you can't afford to buy these instruments. Whom should you call? Try ORNL.

Our newly created Metrology Research and Development Laboratories facility, one of more than a dozen DOE user facilities at ORNL, is making some of the best and most precise measurement instruments in the world available to representatives of industry and universities. Use of our instruments enables small companies to expand their capabilities, but they also benefit large companies from around the nation.

We offer access to unique instrument arrays in research centers for developing and testing measurement and sensing technologies. Here you can measure temperature; flow rate for liquids and gases; light intensities and diffraction; and electromagnetic, acoustic, and ionizing radiation levels.

One unique instrument available is the gravimetric calibrator, a state-of-the-art device that can measure flow rate of any type of gas. Built for use by the semiconductor industry, it has been awarded an international patent and received an R&D 100 Award from *R&D* magazine in 1995.

We offer the capability to measure electrical noise that might interfere with operation of electronic systems. Such testing can be done at ORNL or at the user's own facility using portable monitoring equipment loaned by the Laboratory. We also have a facility in which a user can expose equipment to harsh industrial environments for long-term tests. Such experiments can be controlled remotely over the Internet.

The Metrology Research and Development Laboratories also offer more than 40 years of expertise to users. ORNL has more than 100 scientists and engineers who specialize in diverse areas of measurement and sensor technology. Many also develop new measurement and testing techniques. Our capabilities should measure up to industrial expectations.

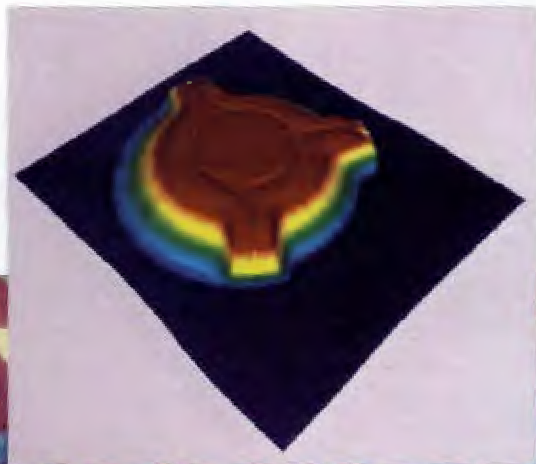
ORNL Helps the Metals Industry

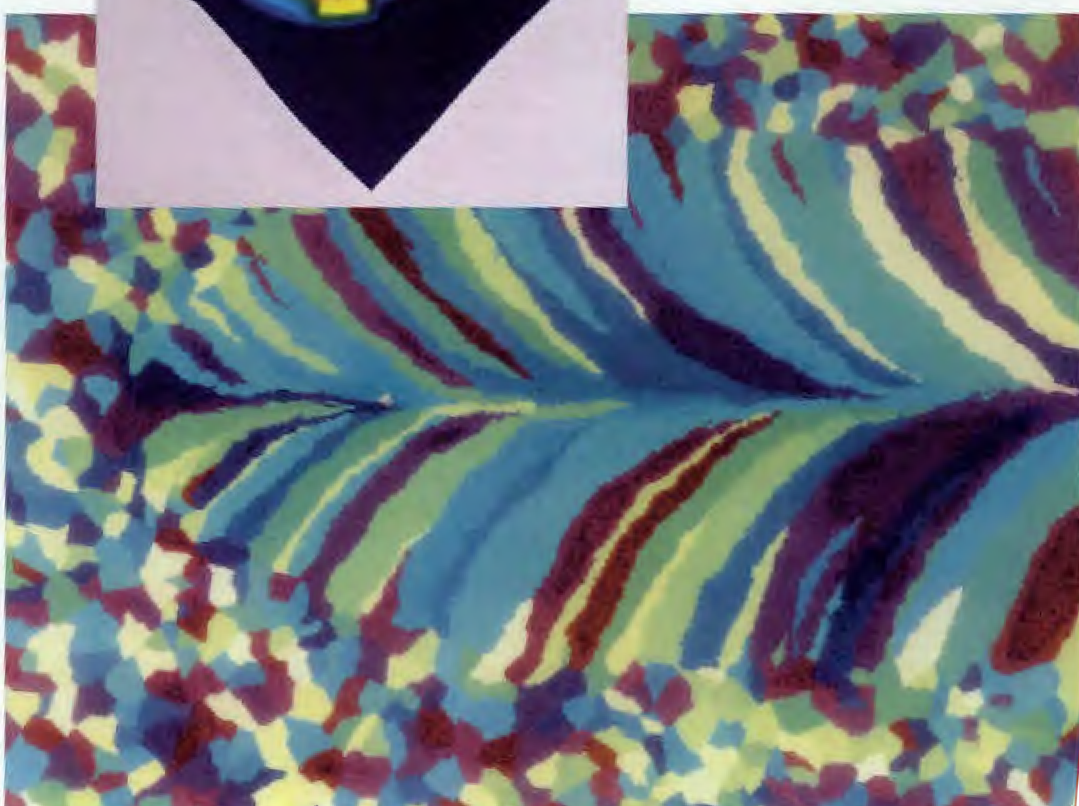
Although the U.S. metals industry is one of the most advanced in the world, there is still room for improvement. By taking advantage of specialized technical expertise and equipment at ORNL, for example, industry could find ways to use less energy and release less pollution in its processes, saving money and jobs and becoming more competitive.

Recently, a company in Georgia found that use of ORNL-developed nickel aluminide for rails in its walking-beam furnaces made possible the commercializion of this furnace technology. The furnaces are used to soften steel bars for making tools. Thanks to the high-temperature strength of nickel aluminide, the furnaces can provide rapid heating, using less natural gas and process cooling water. Because this technology reduces energy use and emissions, it should enable U.S. companies to be more competitive and to save jobs. This kind of assistance is available to the aluminum, chemical, forest products, foundry (metal melting and molding), glass, petrochemical, and steel industries. It is offered through the Metals-Processing Laboratory User Center (MPLUS), a DOE user facility at ORNL.

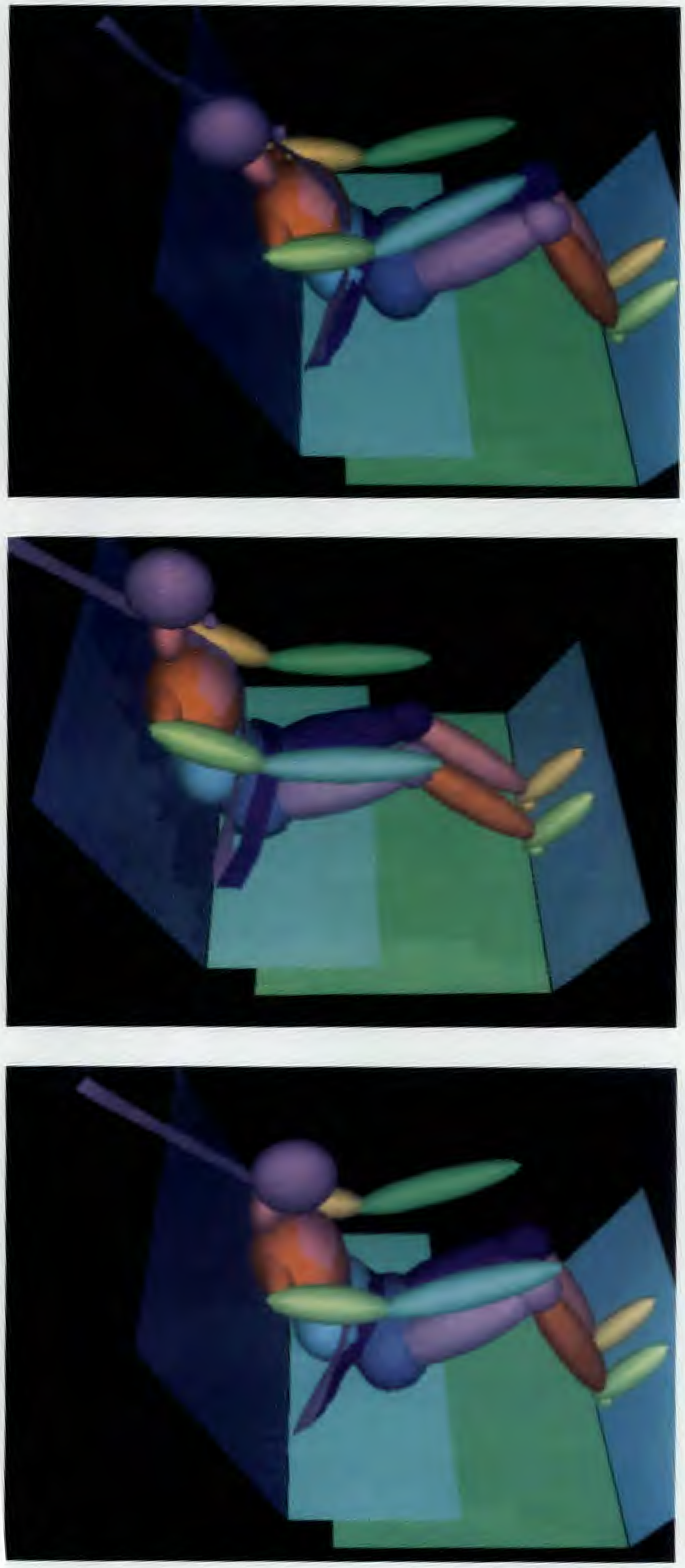
To help industry adjust to rapid changes in the marketplace and improve products and processes, MPLUS offers the services and equipment of its four centers:

- **Metals processing**—casting, powder metallurgy, deformation processing (forging, rolling, and extrusion), melting, thermomechanical processing
- **Metals joining**—welding, monitoring and control, solidification, brazing, bonding, weld modeling





Computer simulations of deformation (top) and solidification as a result of metal processes are some of the services of the Metals-Processing Laboratory User Center.



Our Metals-Processing Laboratory User Center should help U.S. industry become more competitive.

- **Metals characterization**—corrosion, fracture mechanics, mechanical properties, microstructure, nondestructive examination, properties database
- **Metals process modeling**—mathematical design and analysis, solidification, microstructural evolution, and high-performance computing (which can do crash simulations of new designs of cars to determine if the designs and materials used meet safety standards).

The MPLUS Center provides industry with access to the expertise of our partners such as universities, other DOE laboratories, and internal facilities—the High Temperature Materials Laboratory (including the Residual Stress User Center), Computational Center for Industrial Innovation, and the Oak Ridge Centers for Manufacturing Technology. We make room for industry to help it compete.

The MPLUS User Program is supported by DOE, Office of Energy Efficiency and Renewable Energy, Office of Industrial Technologies. ornl

The effect of a car crash on a dummy is simulated by the Intel Paragon XP/S 150 supercomputer at ORNL. Simulations of car collisions are performed for MPLUS.

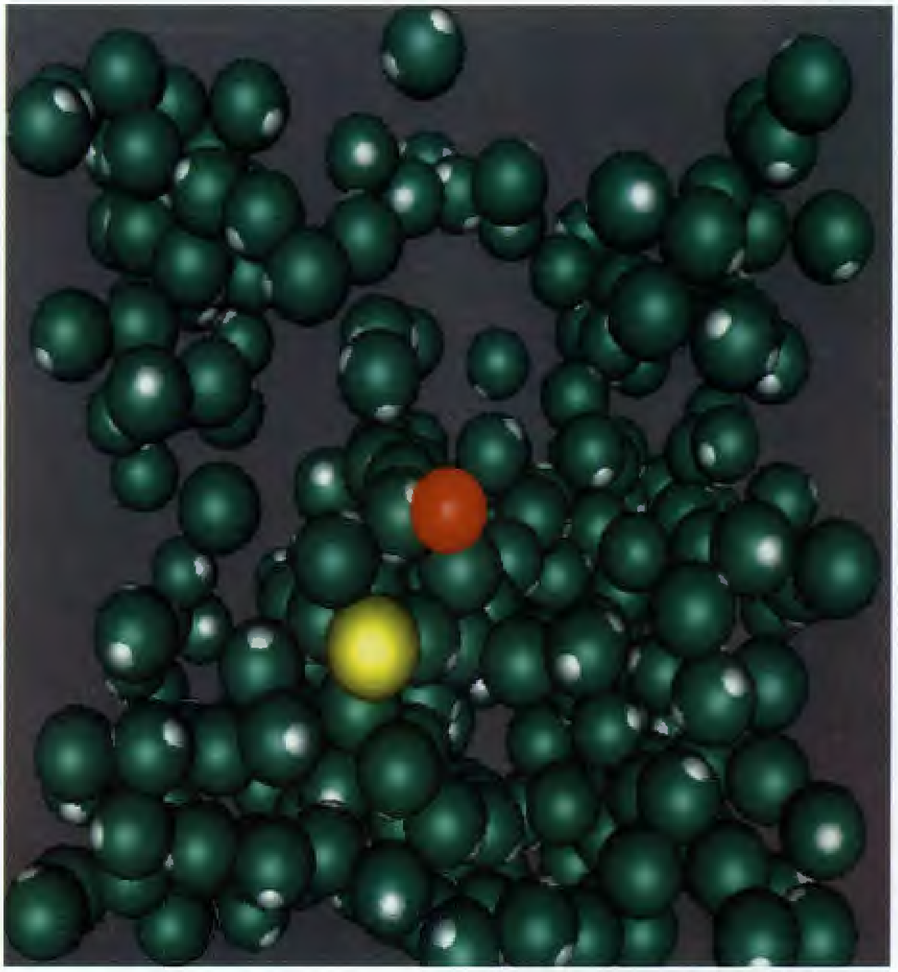
R&D Integration and Partnerships

To get more bang for the buck, we are integrating our internal research activities and setting up partnerships with external research organizations. In these ways, we can leverage and broaden our science and technology programs.

Research and development (R&D) integration is achieved through coordinated program planning, co-location of basic and applied programs within research divisions, and interdisciplinary teaming in mission areas. Each ORNL core competency represents an integration of as many as a dozen major R&D programs ranging from basic research through applications and technology transfer.

R&D partnerships with universities, industry, and other government laboratories strengthen and extend Laboratory programs while making more efficient use of technical resources and facilities. These partnerships include research collaborations, guest scientists and personnel exchanges, shared access to unique facilities, cooperative agreements with industry, and special relationships with other DOE facilities (including the Oak Ridge Y-12 Plant and K-25 Site), the University of Tennessee at Knoxville (UTK), the Tennessee Valley Authority (TVA), and other institutions.

In recent years, R&D partnerships at ORNL have significantly increased. Approximately 35% of ORNL research publications now include authors from other institutions, up from 20% five years ago. The number of guest scientists who perform research at the Laboratory has nearly doubled in 5 years. We host more than 2000 university and 1500 industry researchers per year. We maintain particularly close ties with UTK; through cooperative arrangements such as the ORNL/UT Science Alliance, more than 100 UTK faculty and graduate students perform research annually at ORNL. More than 160 CRADAs have been executed since 1990, representing $170 million in cooperative research with our industrial partners.



Molecular simulation of sodium and chloride ions (red and yellow spheres) dissolved in supercritical water (green spheres), a high-temperature, high-pressure, fluid state of water that makes a salt (such as sodium chloride) much less soluble than it is in normal liquid water. Understanding this phenomenon may aid the design of processes for destroying organic wastes using supercritical water as the solvent.

Creating Products By Modeling Molecules

ORNL has two world-class capabilities that could make a world of difference to industry. We can now

Through the new Joint Institute for Molecular-Based Engineering and Science, ORNL and UTK will combine molecular-level computation with neutron scattering results to help industry design better products.

model molecules, using powerful parallel computers. We have long been able to scatter neutrons from a target in our HFIR to probe a material's structure. Combining these capabilities, we can get for the first time a coherent picture of molecules or molecular-level processes responsible for properties such as unusual strength or the ability to fight disease.

What's in it for industry? We can help design a synthetic motor oil that will still work when lubricating superhot surfaces in highly efficient engines. We can develop improved computer codes to model enzymes produced by defective genes and design drugs to block these enzymes' harmful effects. Other benefits of molecular simulations may be designs for agents to cleanse polluted water and for environmentally friendly industrial solvents.

Unlocking the subtle mysteries of molecular processes is the key to creating and improving products and processes. Results of neutron scattering experiments have long been relied upon to verify indirectly theories about molecular-level processes. Computers, although useful for modeling atoms and small molecules, lacked the power to simulate large molecules (e.g., polymers) and or complex processes involving many molecules on a scale useful to industry.

Using the Intel Paragon XP/S 150 supercomputer and the special codes we've developed, we can model complex molecular systems of importance to industry. We start with first principles, entering data about atoms and basic molecular interactions. By predicting a new material's properties, perhaps even before the material has been created, we can help industry develop and test new products more quickly and efficiently.

We are studying various properties of natural and synthetic materials at a level of detail previously unimaginable. We plan to develop improved codes to aid in drug design and evaluate etching and coating processes for producing microchips.

Thanks to supercomputers, computation has been elevated to equal status with theory and experiment. Thus, ORNL and the UTK have created the Joint Institute for Molecular-Based Engineering and Science (JIMBES). Combining molecular-level computation with results of neutron and X-ray scattering at ORNL, JIMBES offers a new approach to product development for the world.

The research was supported by ORNL's Laboratory Directed R&D Program.

Center's Tools Aid Environmental Decision Makers

A proposal is made to construct a county landfill near your home. You call a county commissioner and ask if drainage from the proposed landfill would pose a health hazard to your family. You may have identified a complex environmental problem.

ORNL is playing a major role in helping to solve complex environmental problems at local, state, and regional levels as part of the newly established National Center for Environmental Decision Making Research. This center can help decision makers identify an acceptable landfill site by imparting information on successfully used tools and lessons learned in similar situations elsewhere.

To direct the center, the National Science Foundation selected the Joint Institute for Energy and Environment (JIEE), a collaborative research institute involving staff from ORNL, TVA, and UTK, which administers the center. Milton Russell, director of JIEE, professor of economics at UTK, and a collaborating scientist at ORNL, is the center's director. ORNL's Robb Turner is deputy director.

The center assembles specialists who provide decision makers nationwide with the information, techniques, and processes they need to effectively and fairly solve environmental problems. These specialists analyze processes that influence environmental decisions and present the results in a form useful to decision makers. They glean lessons from case studies involving environmental decision making that may apply to other environmental issues. They develop a "toolkit" to guide environmental decision makers facing different situations. They are creating a national source of databases and other information that will be available on the World Wide Web. The center interacts with citizens, leaders in industry, and government decision makers through an outreach program that includes workshops, publications, electronic media, residency programs, conferences, and seminars.

The rationale for the center is that state and local officials and citizens are increasingly being asked to render decisions on difficult environmental issues requiring analysis and information not always readily available. The center's work should result in simpler, faster, and less costly techniques to help local officials make wiser and fairer decisions.

The center should help local officials make wiser and fairer decisions.

Operations and Administration

The day-to-day operation of ORNL is generally the responsibility of the Operations, Environment, Safety, and Health Directorate. We perform the necessary maintenance of infrastructure; provide health services, including physical examinations; assist line organizations in complying with federal and state regulations in such areas as radiological protection, environmental protection, and industrial safety; and provide emergency planning and response. In addition, we provide financial and budget services for all operational and research areas at ORNL and assist divisions with personnel recruitment.

In 1995, as in other years, we found several opportunities for cost savings, added efficiencies, and more innovative ways of doing business. Here are some examples.

In one example of better resource management, ORNL sent some excess lead to a DOE accelerator in Virginia for shielding.

Lynn Kennedy (left) and a Metler Company employee assist with the loading of lead bricks onto a truck for transport to the Thomas Jefferson National Accelerator Facility in Virginia. *Photograph by Jim Mottern.*

ORNL Recycles Excess Lead

To keep worker exposures to radiation as low as reasonably achievable in ORNL reactor and accelerator experiments, lead is used as shielding. Since June 1989, because ORNL's Lead Shop had suspended operations and lead has been procured from external sources, the Laboratory has accumulated 3.9 million pounds of excess contaminated and uncontaminated lead.

A team was established in January 1995 to address health, safety, and environmental concerns in managing our lead inventories. The task team accomplished the following:

- Completed the "ORNL Lead Management Plan," which addresses procurement, exchange, tracking, use, storage, decontamination, internal and external processing, and disposal of waste lead.

We dismantled and cleaned 24 chemical fume hood ventilation systems contaminated with perchlorate salt.

Barry Gaskins (left) and Howard Sneed prepare a hood fan for a bath to remove its perchlorate salts.

- Reopened ORNL's Lead Shop on October 1, 1995, for lead recycling. This shop is accepting noncontaminated, "green-tagged" lead from Laboratory operations no longer needing it and sending low-level contaminated lead bricks to ORNL's Physics Division for shielding.

- Planned and executed the transfer of 120 tons of uncontaminated lead bricks to DOE's Thomas Jefferson National Accelerator Facility (TJNAF) in Newport News, Virginia. Noncontaminated lead from our closed-down Tower Shielding Facility reactor was also sent to TJNAF for shielding.

This transfer of lead between two DOE facilities, the first of its kind in DOE history, was a sensible act. Because lead is both a toxic metal and a valuable shielding material, it is more economic to reuse it as shielding where needed than to dispose of it as waste. Through the transfer, ORNL saved about $660,000 in one year in potential disposal costs. It also prevented the possibility that employees might be exposed to unmonitored and improperly stored lead. In minimizing waste disposal while making effective use of waste lead, ORNL has led the way.

The lead recycle work was supported by TJNAF.

Hoods Cleaned and Reinstalled

In 1990, an ORNL industrial hygienist discovered that hot perchloric acid had been used in a laboratory hood, a protective enclosure that ventilates noxious fumes, dust, and gases so that biological, chemical, and radioactive materials can be safely handled. She reported the problem. When additional investigation found that the chemical had been used in other hoods also not approved for hot perchloric acid, Laboratory management recognized a safety problem and responded swiftly.

In 1995, ORNL's Office of Safety and Health Protection successfully completed the project to dismantle and decontaminate 24 chemical fume hood ventilation systems contaminated with perchlorate salt. The clean hoods were then reinstalled. The threat of fires and explosions in these systems was eliminated, and all hoods met environmental, health, safety, and radiation limits.

The project finished three months ahead of schedule, saving ORNL $6 million in costs avoided in putting hoods in compliance when returned to operation in the labs. By following procedures and reusing two-thirds of the decontaminated ductwork and system materials, we significantly reduced the discharge of liquid and solid waste from the cleanup effort.

The work was sponsored by DOE, Office of Energy Research.

Declining Work Force Heightens Emphasis on Human Resources

ORNL's recruiting activity during 1995, though limited, focused on filling openings created by retirements.

Following the 1994 Special Retirement Incentive Program when 429 ORNL employees elected to retire, the Laboratory work force has continued to decline. Although about 30% of those employees were replaced in 1995, changing budgets in specific programmatic areas have further reduced staff levels. This decline should not be construed, however, as a diminished commitment—at corporate, customer, or Laboratory level—to the development and management of human resources. If anything, it has prompted ORNL to reaffirm its goal to recruit and retain the staff needed to achieve programmatic goals. Consequently, activities in staff recruiting, retention, and diversity have been refocused or intensified.

ORNL's recruiting activity during 1995, though limited, focused on filling openings created by retirements. Of these openings, 131 were filled—88 through internal transfers and 43 by outside hires. Both transfers and hires were conducted in keeping with the Laboratory's equal employment opportunity (EEO) and affirmative action (AA) goals. Complementing these endeavors were efforts to increase the cultural diversity of ORNL's work force. Participation in the National Consortium for Graduate Degrees for Minorities in Engineering and Sciences, Inc., for example, resulted in the hiring of three staff members. During the summer of 1995, a partnership with the Southeastern Consortium for Minorities in Engineering produced positions for seven interns.

In an effort to retain staff essential to ORNL missions, the Employee Development Task Team was chartered to take a critical look at employee development opportunities at ORNL and to suggest enhancements. The team reviewed and considered issues identified from two employee surveys and an assessment by the human resources consulting firm Watson Wyatt. Issues identified include developmental assignments, mentoring, and job rotation. In addition, the task team designed a survey for identifying best practices and is currently conducting the survey with five companies. Adapting those best practices to the Laboratory culture, analyzing and applying lessons learned from the internal surveys and assessments, and meeting EEO/AA and diversity challenges—all will receive special emphasis in ORNL's strategic planning for human resources.

New Focus on Performance, not Compliance

Interested in establishing a reenergized and progressive relationship with your customer? If so, take note of the Business Management Oversight Pilot (BMOP) recently implemented at the Laboratory for ORNL and its then contract manager Lockheed Martin Energy Systems (LMES). Described in Deputy Secretary of Energy Charles Curtis's memorandum of March 30, 1995, BMOP makes possible a type of partnership between DOE and the contractor that encourages and rewards performance and continuous improvement. It does so by facilitating a paradigm shift from compliance-based to performance-based oversight.

The initial step in implementing BMOP here was to schedule a two-week DOE-ORO review, which will be part of a cyclical process. This year's review was set for February 12–23, 1995. The next step was to develop a set of performance objectives and measures mutually agreed to by LMES and ORNL managers and their DOE counterparts. From this cooperative effort emerged 23 objectives and 66 measures against which LMES-ORNL later assessed its own performance. Using both the self-assessment and evidence of operational awareness gleaned from routine communications and interactions, DOE-ORO determined the scope of the on-site review. Protocol for the review called for an entrance conference, regular meetings with LMES-ORNL management during the review, and an exit conference. The review findings formed the basis for a report to the Deputy Secretary of Energy. Eventually the findings will result in corrective actions and improved performance objectives and measures. Then the cycle will begin anew.

The expected benefits of this new partnership with DOE are many. The annual process of determining and agreeing on performance objectives and measures should not only improve communications among LMES, ORNL, and DOE managers but also facilitate the self-assessment process. Replacing several on-site reviews and assessments with one annual review should reduce the level of staff support required and result in significant cost savings. Moreover, further cost reductions and avoidances should be realized as operations incorporate best management practices. Most important, by establishing and maintaining their own management systems for monitoring and achieving expectations, LMES and ORNL can ensure that performance and process improvements are continuous. This process should also ensure that the paradigm shift does not reverse itself.

The annual process of determining and agreeing on performance objectives should improve communications among managers and facilitate self-assessment.

Presentations to DNFSB Staff Successful

Four staff members of the Defense Nuclear Facilities Safety Board (DNFSB) visited the Laboratory March 13-15, 1995, to receive a general overview of ORNL's nuclear facilities and inventories. Arrangements for the visit were coordinated through the Office of Operational Readiness and Facility Safety. Presentations made by managers of various ORNL facilities focused on the operational and programmatic history and the current nuclear material inventory for 14 operational and 12 shutdown facilities. Following the presentations, the DNFSB staff members participated in brief tours of 19 facilities.

Prior to their visit, the DNFSB staff had requested that presentations address plans for the disposition of nuclear fuels and radioactive materials, configuration and form for stored nuclear materials, and DOE programmatic ownership of nuclear materials inventory. They had also expressed interest in radiation and contamination levels within facilities and in plans for the decontamination and decommissioning of shutdown facilities.

At the end of their visit, the DNFSB staff expressed satisfaction that ORNL had paid close attention to their desired agenda and had provided the kinds of information requested. Their comments were complimentary of the professionalism, confidence, knowledge, and capability of the Laboratory staff. The best indicators of success, however, may be that all DNFSB-initiated issues were resolved during the visit and that follow-up was not anticipated.

Radiation Protection Office Award

The ORNL Award of Excellence in Operations and Support in 1995 went to the Office of Radiation Protection (ORP). The award recognized the office's demonstrated excellence in providing effective, efficient radiation protection support to the Laboratory and improvements in the overall radiation protection program.

One outstanding achievement for which ORP was cited was the complete revision of the ORNL *Health Physics Manual*, to comply with federal standards, and DOE's *RadCon Manual*. The award also honored ORP for performing a detailed Malcolm Baldrige assessment and customer surveys to provide more customer focus, implementing positive changes, and developing performance measures to monitor effectiveness of those changes. Moreover, ORP was commended for the downward trend in overall radiation dose received by the Laboratory population.

Closing in on Compliance

During 1995 ORNL's environmental compliance personnel focused on two major undertakings, making significant progress in both. One effort involved federal and state regulations governing underground storage tanks (USTs) and the other involved negotiations to renew DOE-ORO's National Pollutant Discharge Elimination System (NPDES) permit.

To respond to UST regulations, we facilitated the closing of nine petroleum tanks at ORNL and received approval letters for final closure of an additional six. This achievement represents a significant step toward closing or upgrading all petroleum tanks by the end of 1998, the deadline set by state and federal regulations. By then all existing USTs must comply with operating standards for new tanks. In addition, investigations of soil and groundwater must be conducted during all tank closures and when a petroleum release is suspected or confirmed.

The program, involving staff from several ORNL divisions, was created to ensure that the deadline is met and to facilitate the inevitable soil and groundwater investigations. The Laboratory chose the team approach to avoid burdening individual research divisions with undue liability for "legacy" tanks and to enable application of lessons learned to successive tank closures, replacements, and site investigations. With 42 of ORNL's 55 tanks now closed and 3 relatively new ones already meeting regulatory standards, the team is confident that the remaining tanks can be closed and full compliance achieved by the deadline.

Our compliance people also facilitated negotiations to renew DOE-ORO's NPDES permit. Discussions are still under way with staff from the DOE Site Office and the Tennessee Department of Environment and Conservation. Having qualified for all prerequisites, ORNL has been operating under the conditions of the previous permit, which expired in 1991. We are negotiating a permit that is more relevant to 1996 ORNL operations, enables implementation within restricted budgets, and ensures the best possible chance for full compliance. Where stricter requirements may be imposed, the team is proposing feasible alternatives. Where alternatives are not available, achievable schedules for compliance with new requirements are being suggested.

One benefit may be that less DOE oversight, made possible by ORNL's self-monitoring, will result in continuous improvement in overall ES&H performance.

ES&H Oversight: Will Less Mean More?

To increase the efficiency and effectiveness of DOE's oversight of our environmental, safety, and health (ES&H) activities, the Department decided to explore alternatives to its current way of doing business. The ES&H Oversight Reduction Pilot at ORNL, one of three pilots accepted by DOE, was an outcome of DOE's decision to change its approach. Initiated in an August 31, 1995, memorandum from Deputy Secretary of Energy Charles Curtis, the pilot is meant to demonstrate that oversight based on performance, rather than compliance, can significantly improve contractor performance while actually reducing the number of DOE reviews. The pilot is based on a set of performance measures mutally agreed upon by DOE and ORNL. Negotiation of these measures, which are in addition to ES&H measures already built into LMER's new performance-based contract, was the first phase of the pilot oversight process. The second phase involved continuous baselining of ORNL's performance against performance data from prior years, assessing performance against the negotiated measures, and providing monthly progress reports to DOE. The monthly reports were followed by quarterly discussions of progress and then a yearly comprehensive self-assessment by the Laboratory. Finally, during a two-week period in August 1996, an ES&H appraisal of ORNL by all DOE programs, coordinated by DOE-ORO, will be conducted on-site. The scope of the review will be affected by monthly performance indicators, ORNL's self-assessment, and any external reviews.

Besides the August appraisal, no other ES&H oversight of ORNL activities should be conducted by DOE programs throughout FY 1996. Possible exceptions might be independent reviews conducted by Environmental Health or reviews prompted by serious deficiencies in meeting performance measures. The success of the pilot oversight, made possible by ORNL's self-monitoring, will result in continuous improvement in overall ES&H performance.

Jim Duncan (left), Kent Francis, and O. C. Duck assemble a projectile fuse conveyor for the Advanced Integrated Robotics Rearm System.

Crafts Workers Aid Success of Army Project

Some assignments involving our skilled crafts workers are both challenging and exciting and contribute to important initiatives originating outside the Laboratory. One recent project for the U.S. Army, for example, required fabrication and assembly of components for the Advanced Integrated Robotics Rearm System (AIRRS), designed by ORNL researchers. As a proof-of-principle activity, AIRRS demonstrated the feasibility of automated processing of artillery rounds on board the Army's Future Armored Resupply Vehicle. Crafts workers were initially involved in AIRRS for the fabrication of system components. These included computers, servo motors, pneumatic actuators, and a wide variety of sensors working in unison to move, process, and store artillery projectiles and fuses. Once fabricated, they had to be mounted and integrated into the system. These tasks were expertly handled by our electricians, millwrights, pipefitters, and welders. Working alongside the engineers and technicians, our crafts personnel provided valuable insights and recommendations that enhanced the reliability of the system. When AIRRS was successfully demonstrated in September 1995, the crafts workers were justifiably proud of their significant contributions to this national security project.

Working alongside the engineers and technicians, our crafts personnel provided valuable insights and recommendations that enhanced the reliability of the Advanced Integrated Robotics Rearm System.

Other Highlights of Laboratory Operations

- Lockheed Martin Transportation and Packaging Management hosted the 31st Annual Contractors Transportation Management Association Conference. Over 130 participants attended, including representatives from 24 contractors, 7 DOE field offices, 5 regulatory agencies, 24 vendors, and DOE Headquarters.

- An ORNL Compliance Assurance Program was established to ensure an effective coordination of Price-Anderson and Standards Management activities.

- The Office of Operational Readiness and Facility Safety coordinated development of a multiprogram implementation plan to comply with DOE Orders 5480.22B and 5480.23 for the revision to ORNL Technical Safety Requirements and Safety Analysis Reports.

- The External Dosimetry Program was found to be without deficiency and was reaccredited for two years by the DOE Laboratory Accreditation Program.

- The security of the High Flux Isotope Reactor and Tower Shielding Facility reactor was recategorized, resulting in a reduction of security costs there. Additional badge readers at rotogates were installed, providing easier and less costly access.

- The Office of Quality Programs and Inspection provided inspection and engineering support for a Work-for-Others contract with the Department of Transportation, Office of Pipeline Safety. Inspection and engineering personnel have been on site in various states to witness pipeline construction or repair activities.

- Plans were developed to install dechlorination systems for several untreated ORNL release points. Chlorine removal is required in the proposed National Pollutant Discharge Emission Standard permit for ORNL with the state of Tennessee.

- The Plant and Equipment Division established a program for recycling fluorescent light tubes.

- An advanced computing platform that tracks the inventory of radioactive material within a nuclear facility was designed and implemented in partnership with the University of Tennessee at Knoxville.

Technology Transfer: CRADAs, Licenses, and Patents

Oak Ridge National Laboratory has one of the most successful technology transfer programs in the DOE system. The Oak Ridge program, managed by Lockheed Martin Corporation's Office of Technology Transfer in Oak Ridge, leads the DOE complex in the number of cooperative research and development agreements (CRADAs) and licensing agreements and in total licensing revenues and extent of industrial outreach. Since 1990, ORNL has entered into 163 CRADAs (52 in 1995) with a total value of $132 million. ORNL has also executed 128 licenses since 1985 (36 in 1995), resulting in over $100 million in sales and generating more than $3 million in royalties for use in technology transfer activities. Sales of licensed products in 1995 increased by 35% over the previous year. Patent applications have more than tripled in the past 5 years and are approaching 100 per year.

An important component of the ORNL technology transfer effort is the Energy Research Laboratory Technology Research (ER-LTR) Program, which is managed by the Office of Science and Technology Partnerships (Partnerships Office). This program seeks to capitalize on ORNL's multidisciplinary strength by supporting research that enhances its mission, as well as providing the technological underpinnings needed for the future growth of American industry. Within this framework, research is being performed in support of the development of three critical national technologies: advanced or tailored materials, intelligent manufacturing, and sustainable development (energy, environment, and biotechnology). This effort is accomplished through technology research and maturation projects and cost-shared collaborations such as CRADAs, personnel exchanges, and technical assistance projects.

Currently, the ORNL portfolio includes 35 multiyear projects, 21 single-year CRADAs, five technology maturation projects, two personnel exchanges, and 52 technical assistance projects. Nearly half of the CRADAs and over 80% of the technical assistance projects involve small U.S. businesses. The Laboratory Technology Research Program offers an effective and appropriate mechanism for federal investment in cost-shared R&D. Clearly, this type of joint investment capitalizes on two great strengths: the world-class research capability of ORNL and the unparalleled entrepreneurial spirit of American industry.

The following tables provide information on ORNL involvement with private firms through CRADAs, ORNL technologies licensed to industrial firms, and ORNL staff patents for 1995.

CRADAs Executed in 1995 in Oak Ridge

Client	Technology	Principal Investigator(s)
Low Emissions Technologies Research & Development Partnership (USCAR)	Cylinder design for reduced emissions origins	Ronald L. Graves
RhoMed, Inc.	Rhenium-radiolabeled antibodies and peptides for cancer therapy	F. F. (Russ) Knapp
GelTech, Inc. (resubmitted)	Novel cost-effective process for the replication of hybrid diffractive-refractive optical elements in silica glass	Bruce E. Bernacki, L. Curt Maxey
Metal Matrix Composite Castings, Inc.	Fabrication of cast metal matrix components	James G. Hansen
Hoskins Manufacturing Co.	Development of commercial applications of FAPY (iron aluminide) alloy	Vinod Sikka
Cummins Engine Co.	Study of bonding interfaces between reinforcing materials and cast aluminum alloys	Karren More, Ted Nolan, Vic Tennery
International Sensor Technology, Inc.	Development of protocols using thermoluminescent detector arrays for two-dimensional mapping of alpha activity on surfaces and in soils	Richard B. Gammage
Fiber Materials, Inc.	Carbon-carbon composite orthopedic prosthesis and implants	Tim Burchell
USCAR(AMP)	Rapid tooling for functional prototyping of metal mold processes	Thomas Zacharia
USCAR(AMP)	Design and product optimization for cast light metals	Srinath Viswanathan
Interscience, Inc.	Ultraprecision automated measurement for manufacturing	C. E. Thomas
Engelhard Corp./ICC	Moving advanced desiccant materials into mainstream non-CFC cooling products	Philip D. Fairchild
Hughes Christensen/Houston Advanced Research Center	Implantable incipient failure monitor for use in certain oil field drill bits	David Holcomb
Remtech	Efficient on-site degradation of high concentrations of spent deicing fluids	Janet Strong-Gunderson
Marlow Industries, Inc.	New thermoelectric materials for solid-state refrigeration	Brian C. Sales

Client	Technology	Principal Investigator(s)
Pratt & Whitney	Role of yttrium in improving oxidation resistance in advanced single-crystal, nickel-based superalloys for turbines	Michael K. Miller, Edward A. Kenik
Narlron, Advanced Vehicle Systems, Chattanooga Area Regional Transit Authority, Electric Transit Vehicle Inst.	Air-conditioning system with improved efficiency for hybrid-electric vehicles	Don Adams
Teledyne Alvac	Manufacturing nickel-based superalloys with improved high-temperature performance	Chain T. Liu, Easo P. George
Darwin Molecular Corporation	Identification of genes affecting the immune system through studies in mice	Walderico M. Generoso
Southern Technology Council	Establishing the Southeastern Regional Alliance Program in Development of Technology Commercialization	David Jamison
Wolverine Tube Co.	Heat transfer surface augmentation for zeotropic mixture alternatives to HCFC refrigerants	James C. Conklin Van D. Baxter
Occidental Chemical Corp.	Rutherford backscattering analysis of the failure of chlorine anodes	Catherine E. Vallet, Ray A. Zuhr
USCAR (LEP)	Powertrain sensors and actuators: materials, design, process modeling	William L. Bryan
Advanced Ceramics Research	Rapid prototyping of bioceramics for implants	Ogbemi O. Omatete
Ford Motor Company	Engine control improvement through application of chaotic time series analysis	C. Stuart Daw
Nomadic Technologies, Inc.	Improved design of the omnidirectional robotic platform for enhancement of manufacturability and commerciability	Francois G. Pin
Tennessee Resource Valley	Development of a technology strategy for the state of Tennessee	Bill Eads
Reynolds Metals Co.	Development of aluminum bridge deck system	Wayne Hayden
PerSeptive Biosystems, Inc.	Laser desorption time-of-flight mass spectrometer DNA analyzer	C. H. Winston Chen
Hyper-Therm High-Temperature Composites, Inc.	Optimization of porous silicon carbide fiber coatings	Edgar Lara-Curzio Karren More
Textile Research Institute (AMTEX)	On-line process control project	Eric Wachter

CRADAs Executed in 1995 in Oak Ridge

Client	Technology	Principal Investigator(s)
Physio-Control Corporation	Heart pathology determination from electrocardiogram signals by application of deterministic chaos mathematics	Ned Clapp
Doehler-Jarvis Corporation	Manufacture of die-casting dies by hot isostatic pressing	Srinath Viswanathan
Lambda	Microwave processing technology development	Robert Lauf
The Aluminum Association, Inc.	Evaluation and prevention of molten aluminum-water steam explosions in casting	Rusi Taleyarkhan
Moftech Corporation	Application of ceramic electrolyte thin films in lithium polymer batteries	John B. Bates
Alumax Technology Corp., Kaiser Aluminum & Chemical Corp., Reynolds Metals Co.	In-line sensors for electrolytic aluminum cells	Jack Young
Thompson Aluminum Casting	Metal compression forming of aluminum alloys and metal matrix composites	Srinath Viswanathan
International Road Dynamics, Inc.	Advanced weigh-in-motion system for weighing vehicles at high speeds	Jeff Muhs
RIS Corp.	Monolithic circuits for barium fluoride detectors used in nuclear physics experiments	James R. Beene
Aerometrics, Inc.	Development and evaluation of a lateral position lane tracking system	Richard J. Carter
Cryo Dynamics, Inc.	Energy-efficient and environmentally friendly surface-cleaning system using carbon dioxide	John R. Haines
Osram Sylvania	Electroluminescent material for flat-panel displays	D. Bart Smith
Thoughtventions Unlimited	Low-loss sapphire windows for high-power microwave transmission	Timothy S. Bigelow
Weyerhaeuser Paper Company	Improved materials for use as components in kraft black liquor recovery boilers	James R. Keiser
AlliedSignal, Inc.	Carbon-carbon composite manufacturing	Tim Burchell
Southwire Co.	Development of superconducting transmission cable	Robert A. Hawsey, Martin Lubell

Client	Technology	Principal Investigator(s)
Teledyne Electronic Technologies	Field deployable continuous monitoring ion trap mass spectrometer	Mike Guerin
Coca Cola Co.	Vending machines using liquid overfeed technology	Vincent Mei, F. C. Chen
Hughes Missile Systems Co.	Gelcasting ceramic defense products	Mark A. Janney

Oak Ridge Technologies Licensed in 1995

Licensee	Technology
Powell River Laboratories	Lead-free bullets (environmentally safe projectiles)
TGM Detectors	Alpha radiation detector
Advanced Systems Technologies Martin Marietta Specialty Components	Active and passive neutron examination and assay system
Tel-A-Train, Inc.	Low-power lasers: "Beware of the Hazards"
Information Systems Planning and Analysis, Inc.	Decision-systems technology
Technology Implementors, Inc.	Environmental screening system
Decision Systems Int'l. Corp.	Hazardous Materials Transportation Expert System
Lambda Technologies, Inc.	Method for curing polymers
SpectRx	Synchronous luminescence system to monitor diabetes
Teledyne Electronic Technologies	Thin-film batteries
Commercial Crystal Laboratories	Superconducting thin films
Applied Poleramic	Electron-beam curing of epoxy resins
Consultec Scientific, Inc.	Microbar and microcantilever sensors for detecting gases, etc.
Tomco Equipment	Cryoblasting
Small Jobs Carpentry, Inc.	Portable microwave instrument for nondestructive evaluation of structural ceramics
Caliper Technologies Corp. and Caliper MicroAnalytic Systems	Microfluidic manipulation for chemical analysis (lab-on-a-chip technology)
Ceramic Magnetics	Gelcasting
AlliedSignal	Fabrication of fiber preforms, structural composite materials
Reynolds Metals, Kaiser Aluminum, Alumax Technology Corp.	Fiber-optic probe
Trane Company	Triple-effect absorption chiller
Genase	Genetically enhanced, cellulase-producing bacterium
United Defense	Nickel aluminide alloys
Merritt Systems, Inc.	Integrated circuit (MaskWorks)
Paradigm IV Technologies	Laser ablation system (optional agreement)

1995 Patents Issued to ORNL Inventors

Inventors	Technology
Tim Scott	Biparticle fluidized-bed reactor
Eal Lee, Lou Mansur, Lee Heatherly	Hard-surfaced polymers
Richard Tyndall	Method that separates bacteria from free-living amoebae
Al Mattus	Submergible torch and method for treating waste solutions
Tim Scott	Electric field-controlled emulsion phase contactor
Curt Maxey, Marc Simpson	Optical wet steam monitor
Tuan Vo-Dinh	Surface-enhanced Raman scattering dosimeter and probe
Tom Kollie, L. H. Thacker, Sandra Fine	Instrument for measuring vacuum in sealed thin-wall packets
Arthur Moorhead, Paul Menchhoffer	Method and apparatus for making articles from particle-based materials
John Bates, Nancy Dudney	Electro-optical device
C. Stuart Daw, Larry Hawk	Fluidization quality analyzer and automatic control loop for fluidized beds
Don Bible, Richard Crutcher, Carl Sohns, Randall Maddox	Handheld microwave instrument for nondestructive evaluation of structures in ceramics
Leon Maya	Maskless laser writing of microscopic metallic interconnect
Don Kroeger, J. Brynestad, C. Hsu	Method of producing superconductor precursors and articles
M. Santella, Gene Goodwin	Nickel aluminide alloys with improved resistance to hot cracking
L. H. Thacker	Gamma-radiation field intensity meter
Bob Lauf, Tom Kollie	Calcium-silicate insulation structure
Lynn Boatner, Janet Rankin, Paul Thevenard, Laurence Romana	Controlled removal of ceramic surfaces with combination of ion implantation ultrasonic energy
Mike Harris, O. Basaran, Tom Kollie, Fred Weaver	Silica powders for powder-evaculated thermal insulating panel and method
Michael Unseren, David Reister	Method for controlling a vehicle with 2 or 4 independently steered wheels
Warren Sisson, O. Basaran, M. Harris	Improved nozzle for electric dispersion reactor
Paul Menchhofer	Fluid casting of particle-based articles
Paul Menchhofer	Casting of particle-based hollow shapes
Eli Greenbaum	Conversion of organic solids to hydrocarbons

1995 Patents Issued to ORNL Inventors

Inventors	Technology
Terry Tiegs, Alice Wittmer	Method of preparing ceramic slurry high in solids and low in viscosity
Charles Forsberg, Edward Beahm George Parker	Reactor accident meltdown limit and control system
Chris Foster, Paul Fisher	Systems and methods for removing unwanted surface layers and producing pellets for cryoblasting process
Kit Haaland	Double-duct liquid metal magnetohydrodynamic engine
Richard Tyndall, Arpad Vass	Methods of degrading napalm and trinitrotoluene
Bill Weaver (3M), David Stinton, Jerry McLaughlin	Flange bonding technique for composite tubes
Barbara Hoffheins, Bob Lauf	Thick-film hydrogen sensor
Doug Lowndes, Jim McCamy	Method for continuous control of composition and doping of pulsed-laser deposited films
Solomon Labinov, Jim Sand	Self-contained small utility system
Rodney McKee, Fred Walker (UT)	Process for growing a film epitaxially upon a magnesium oxide surface and structures formed with the process
Eric Wachter, Thomas Thundat	Microbar sensor
Robert DeVault	Dual-circuit, multiple-effect refrigeration system and method
V. Protopopescu, R. Santoro, J. Tolliver	Fast and secure encryption-decryption method based on chaotic dynamics
David Hobson, William B. Snyder	High-capacity, thin-film rechargeable battery for portable power uses
Hector Lizama, Tim Scott, Chuck Scott	Apparatus and method for desulfurization of petroleum by bacteria

Awards for 1995

ORNL Director **Alvin Trivelpiece** was named chairman of the Science and Technology Advisory Council for the state of Tennessee. He was also named Outstanding Engineer by Region 3 of the Institute for Electrical and Electronic Engineers.

Gerald D. Mahan, ORNL–University of Tennessee Distinguished Scientist, was elected to the National Academy of Sciences.

Gerard Ludtka received the Department of Energy's E. O. Lawrence Memorial Award.

Howard T. Kerr was elected to the Tennesee State Legislature as the 20th District representative.

Herbert A. Mook and **Robert N. Compton** were named senior corporate fellows of Lockheed Martin Energy Systems, and **Malcolm Stocks** was named a corporate fellow. **Compton** also received the 1995 William F. Meggers Award of the Optical Society of America.

For their outstanding computational research on giant magnetoresistance, **Bill Butler, Xiaoguang Zhang,** and **Don Nicholson** of ORNL and **Thomas Schulthess** of DOE's Lawrence Livermore National Laboratory received the DOE-Basic Energy Sciences Division of Materials Sciences Award for Outstanding Scientific Accomplishment in Metallurgy and Ceramics for 1995.

Cyrus Baktash, Chung-Hsuan (Winston) Chen, John W. Cobb, Cullie Sparks, and **Robert B. Warmack** were elected fellows of the American Physical Society.

Tommy Wright was elected a fellow of the American Statistical Association.

Robert M. Westfall was elected a fellow of the American Nuclear Society.

Richard L. Anderson was elected a fellow of the Instrument Society of America.

C. T. Liu was elected a fellow of the Metallurgical Society.

Richard J. Norby, Larry Barnthouse, and **Marvin Poutsma** were elected fellows of the American Association for the Advancement of Science.

Fang C. Chen was elected a fellow of the American Society of Mechanical Engineers.

Ronald L. Beatty, Mark A. Janney, and **David P. Stinton** were elected fellows of the American Ceramic Society.

Ron L. Klueh, Philip J. Maziasz, and **Claudette G. McKamey** were elected fellows of ASM International.

Charles R. Brinkman, John Merkle and **Roger E. Stoller** were elected fellows of the American Society for Testing and Materials.

James F. King was elected a fellow of the American Welding Society.

Robert L. Siegrist was elected a NATO fellow of the NATO Committee on Challenges to Modern Society.

Carolyn Krause was elected associate fellow of the international Society for Technical Communication.

Keith F. Eckerman received a Distinguished Scientific Award from the Health Physics Society.

David E. Reichle was named a member of the Research Coordination Council of the Gas Research Institute.

Phil Jardine was elected chairman of the Soils and Environmental Quality Division of the Soil Science Society of America.

Charles K. Bayne received the 1995 Statistics in Chemistry Award from the American Statistical Association.

Jerome E. Dobson has been elected president of the University Consortium for Geographic Information Science.

Thomas J. Wilbanks received the James P. Anderson Medal of Honor in applied geography from the Association of American Geographers.

Patrick J. Mulholland has been named chair of the Executive Committee of the North American Benthological Society.

A DOE Headquarters Pollution Prevention Award for Technology Transfer for 1995 was presented to **Rick Lowden** for leading the development of lead-free, environmentally safe bullets.

Fang C. Chen and **Vince Mei** have earned the Advanced Technology Award from the Inventors Clubs of America's International Hall of Fame for their invention of a liquid overfeeding air conditioner.

Phillip F. Britt and **A. C. Buchanan** received the Richard A. Glenn Award from the American Chemical Society.

Steve E. Lindberg was recognized by *Science Watch and Current Contents* for authoring one of the Top Ten Hot Papers in Ecology and Environmental Sciences published internationally since 1981.

Ted Besmann was elected vice president for Corporate and External Affairs for the American Ceramic Society.

O. O. Omatete received the Scientific Achievement Award of the National Organization for the Professional Advancement of Black Chemists and Chemical Engineers.

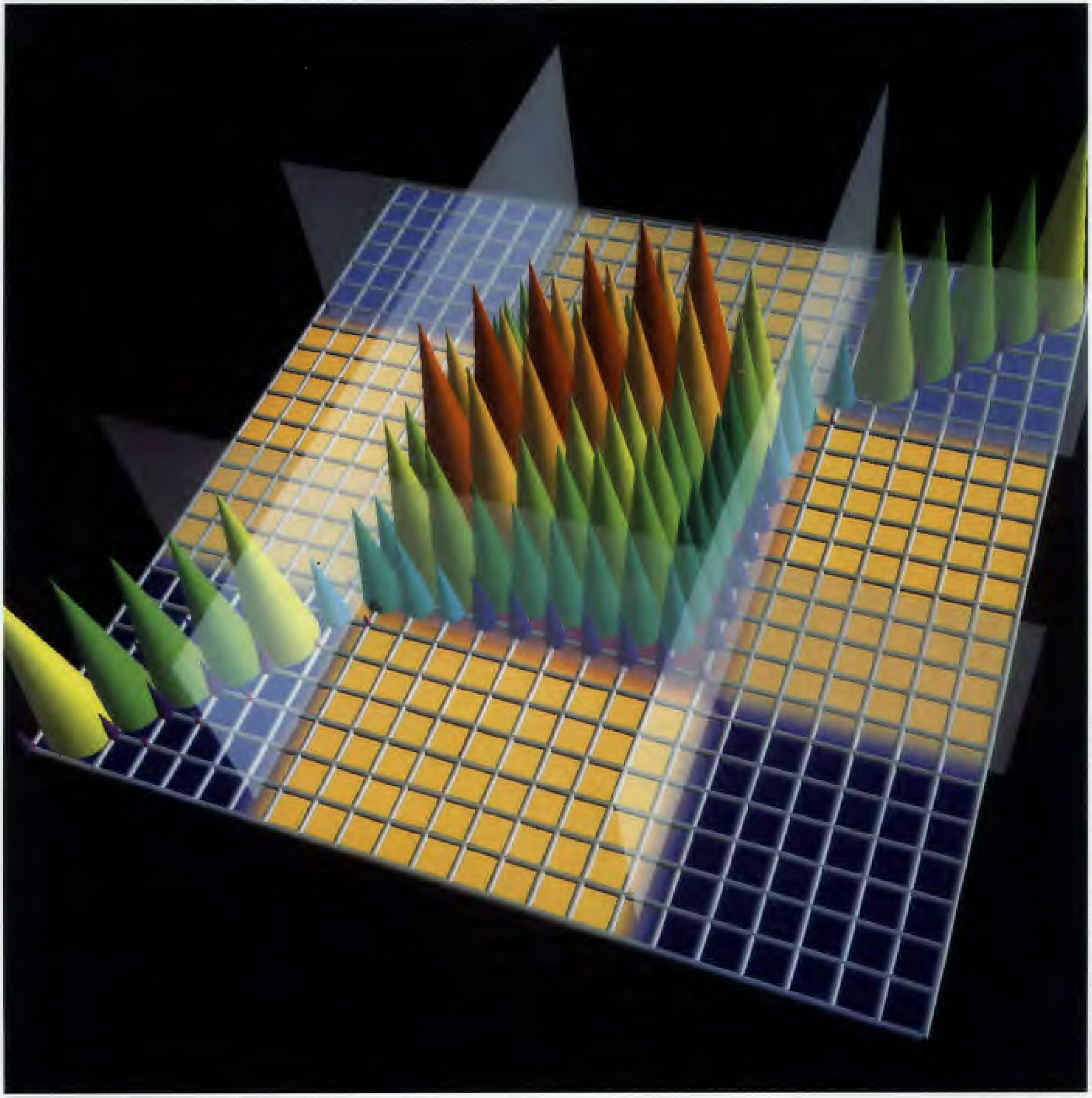
Thomas Zacharia received the William Spraragen Award of the American Welding Society.

ORNL's High Flux Isotope Reactor (HFIR) has received an award from the Nuclear Utilities Service (NUS) for having the most highly rated procedure program among all nuclear reactors at U.S. government facilities.

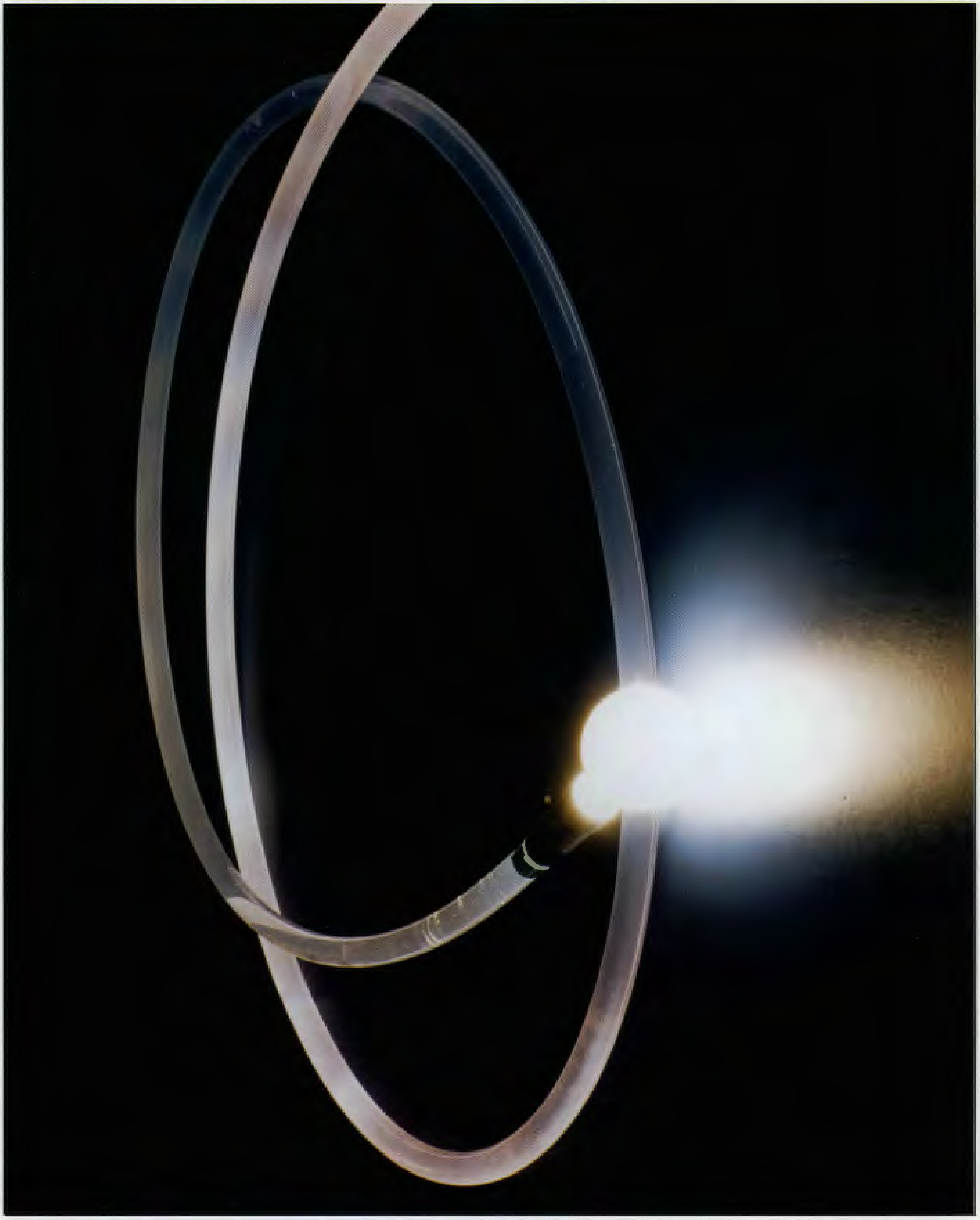
In 1995 ORNL researchers won five R&D 100 Awards from R&D Magazine

Gerald Ludtka received one of DOE's prestigious E. O. Lawrence Memorial Awards in 1995 for his development of the Quench Simulator code to predict the effects of rapid cooling on components.

In 1995 ORNL researchers won five 1995 R&D 100 Awards from *R&D Magazine* in recognition of the year's most significant technological innovations. Four awards were for research done exclusively at ORNL, while the fifth was for a joint entry with 3M Company of St. Paul, Minnesota. Through 1995, ORNL has received 79 R&D 100 awards. The 1995 winners were **Vinod Sikka, Joseph Vought,** and **Seetharama Deevi** (who was on a one-year sabbatical at ORNL from The Research Center, Philip Morris, Richmond, Virginia) for the Exo-Melt™ process, which provides a furnace-loading method for low-cost, energy-saving production of nickel and iron aluminides; **Mark Janney, Ogbemi Omatete, Stephen Nunn,** and **Claudia Walls** for gelcasting, a new ceramic-forming process for making high-quality, complex-shaped ceramic parts; **Carl Remenyik, James Hylton, Timothy E. McKnight,** and **Richard Hutchens** for the gravimetric gas flow calibrator, which can automatically weigh small amounts of corrosive or noncorrosive gases, accurately calibrating gas flow meters such as those used in the semiconductor industry; **Steve Kercel, William Dress, Robert Rochelle,** and **Mike Moore** for the magnetic spectral receiver, which monitors magnetic fields that can affect the function and accuracy of various instruments, including those in nuclear power plant control rooms; and **David Stinton, Rod Judkins, Rick Lowden, Jerry McLaughlin,** and several 3M researchers for the 3M ceramic composite filter, a fiber-reinforced ceramic composite candle filter that removes particulates from hot gas streams in pressurized fluidized bed combustion systems and coal gasification plants, protecting turbine blades needed to generate electricity. **ornl**



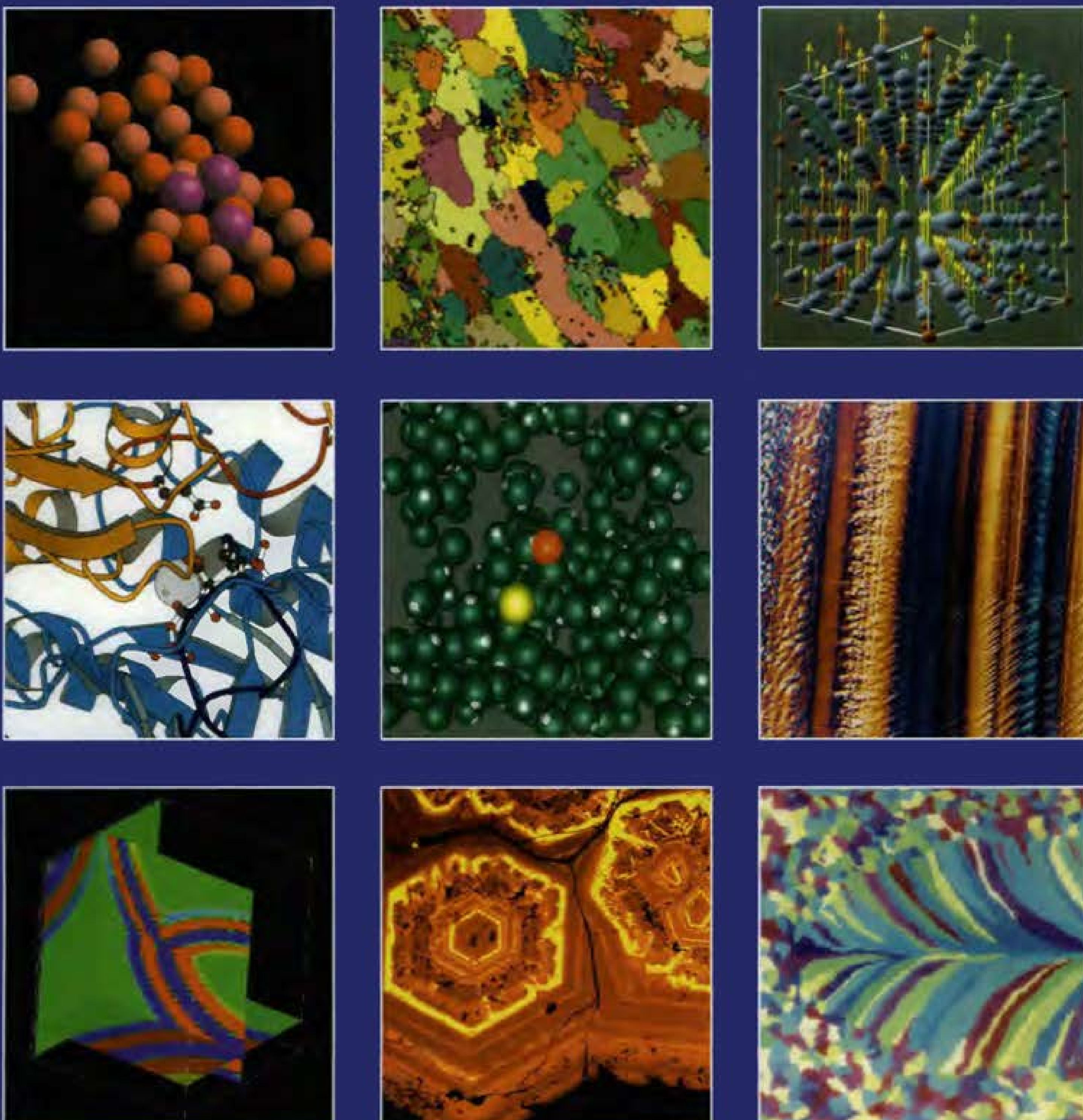
In 1997, a special issue of the *ORNL Review* on high-performance computing using massively parallel processors will be published. It will cover such topics as materials simulations, network research, groundwater modeling, remote operation of research equipment, and simulations of physical phenomena such as melting and giant magnetoresistance in layered magnetic materials. Giant magnetoresistance—a large change in a magnetic material's electrical resistivity caused by an applied magnetic field—is discussed in this issue on pp. 76–77. It is illustrated above in a computer simulation showing electrical conductivity when excess electron spins on cobalt layers are aligned in opposite directions.



The next issue of the *ORNL Review* will explore such topics as biodiversity, biosensors, nuclear medicine, development of a superconducting wire, and hybrid lighting—a combination of natural and artificial illumination to meet indoor lighting needs. Above is a large-core optical fiber that conducts sunlight into a diffusing bulb for indoor lighting.

OAK RIDGE NATIONAL LABORATORY *REVIEW*
P.O. Box 2008, Oak Ridge, Tennessee 37831-6144

U.S. Postage
PAID
BULK RATE
Oak Ridge, TN
Permit No. 3



See inside for the stories behind these images.

POSTMASTER: DO NOT FORWARD: ADDRESS CORRECTION REQUESTED, RETURN POSTAGE GUARANTEED.