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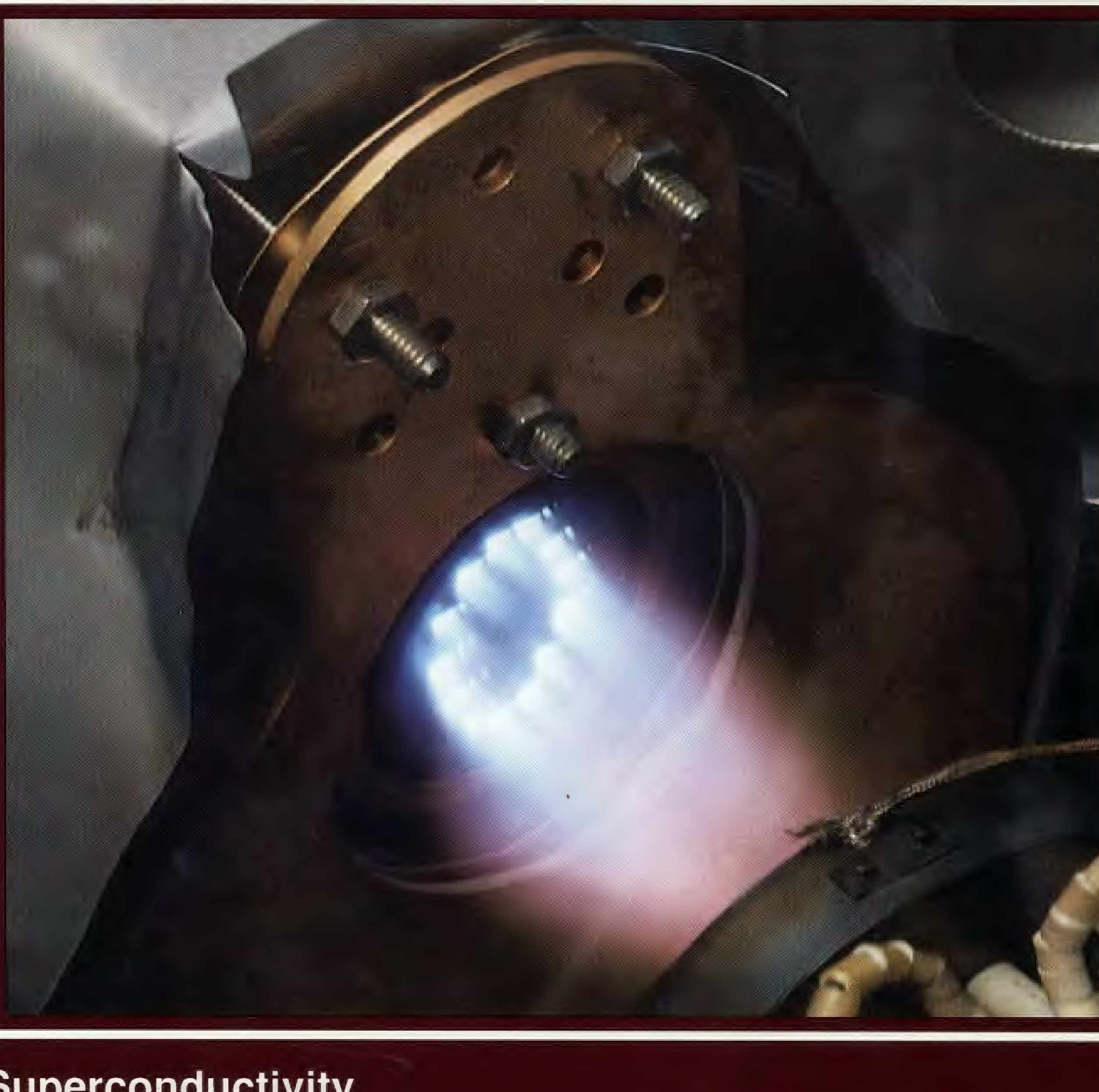
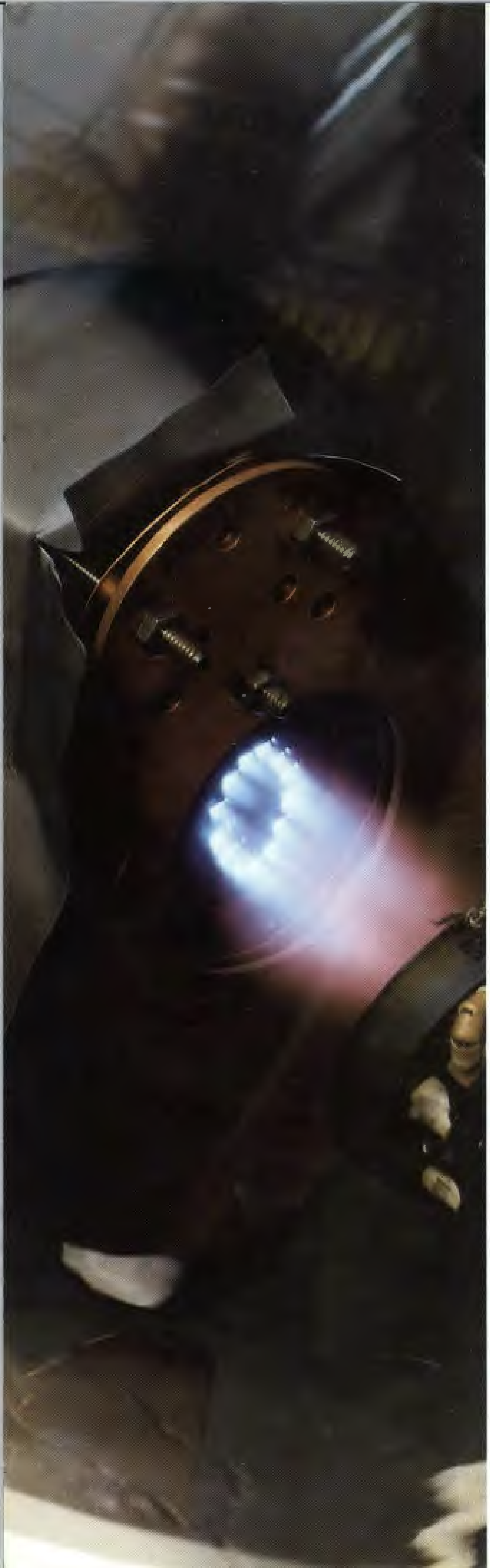


Superconductivity Highlights



ON THE COVER

A pulsed excimer laser beam is scanned rapidly around the surface of a polycrystalline yttrium-barium-copper-oxygen (Y-Ba-Cu-O) target to create a high-velocity plasma, from which crystalline thin films of the high-temperature superconductor $YBa_2Cu_3O_{7-x}$ are grown. The characteristic orange-pink color of the plasma "plume" indicates that yttrium and barium oxides have formed in the plasma and that conditions are correct for growth of high-quality films. This work is conducted in the laboratory of Douglas H. Lowndes of ORNL's Solid State Division. Research on high-temperature superconductivity at ORNL is described in the first three articles of this issue. Photo by Bill Norris.

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REVIEW

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FEATURES

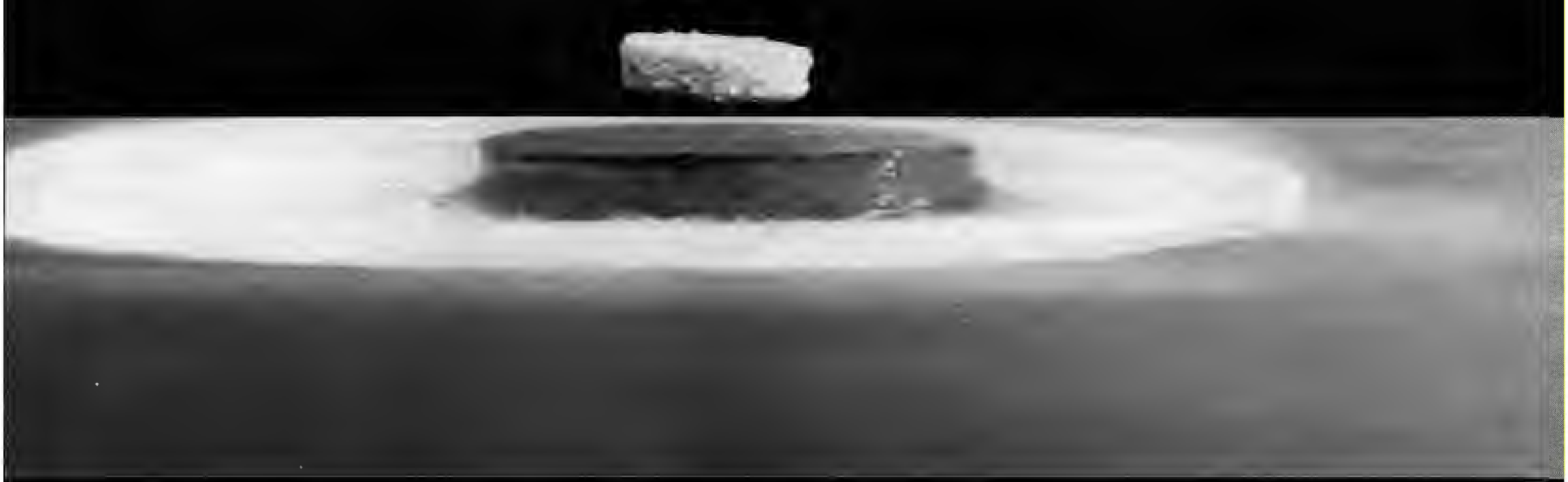
DEPARTMENTS

Oak Ridge National Laboratory is a multiprogram, multipurpose laboratory that conducts research in the physical, chemical, and life sciences; in fusion, fission, and fossil energy; and in energy conservation and other energy-related technologies.

ORNL's High Temperature Superconductivity Pilot Center

An Interview with
Tony Schaffhauser
and Louise Dunlap

HURDLING THE BARRIERS



To find practical applications for the new high-temperature superconducting oxide materials discovered in 1986 and 1987, several barriers must be overcome. Technically, ways must be found to make flexible wires and films from normally brittle ceramic materials that lose all resistance to electrical current when cooled to liquid nitrogen temperatures (75 to 125 K). In addition, for power applications, such as motors and generators, the new materials must be able to carry usable amounts of current in a magnetic field. Researchers are making headway on these problems, as described by ORNL's David Christen in the article on p. 13.

From an institutional point of view, however, other barriers existed. Ways had to be found to speed up the transfer of research results obtained at Department of Energy national laboratories, such as ORNL, to private companies having the ability to manufacture superconducting materials and devices made from them.

Toward this end, DOE in 1988 established High Temperature Superconductivity Pilot Centers at ORNL, Argonne National Laboratory, and Los Alamos National Laboratory (LANL). Pilot Center projects have been jointly developed and cost-shared by industry and government, using new cooperative agreement mechanisms to facilitate cooperation between these parties. To date, the Pilot Center at ORNL has signed 20 cooperative research and development (R&D) agreements with industrial firms.

To learn more about the history, purpose, and progress of the ORNL Pilot Center, the *Review* staff interviewed Tony Schaffhauser and Louise Dunlap, director and former industrial partnership manager, respectively, of the Pilot Center here. An edited version of their comments follows.

Whose idea was it originally to set up High Temperature Superconductivity Pilot Centers at ORNL, Argonne, and Los Alamos?

The idea was originated by Sig Hecker, director of Los Alamos National Laboratory, who suggested it to DOE. Here's the background. In July 1987 President Reagan announced a National Superconductivity Initiative. One part of the initiative established a National Commission on Superconductivity, which published a report in the summer of 1990. He also asked the Defense Advanced Research Projects Agency, the Department of Commerce, and DOE to develop their own superconductivity initiatives. DOE's initiative involved reallocating existing funding for high-temperature superconductivity research. Very little new money was available to put into the effort. DOE also asked its national laboratories to determine how they could work with industry more effectively on this initiative.

So Hecker proposed that LANL set up a Pilot Center for superconductivity and build a facility outside LANL's fence that would be similar to ORNL's High Temperature Materials Laboratory but dedicated to superconductivity. He asked for $25 million from DOE's Energy Research program, which referred him to the Conservation and Renewable Energy program led by Donna Fitzpatrick. She said that new money cannot be easily obtained for bricks and mortar and that DOE labs must use their existing money more effectively. She suggested that Sig talk to people in Oak Ridge who have been effective in technology transfer. Hecker visited Oak Ridge and proposed a joint program involving ORNL and Los Alamos. Argonne National Laboratory also got involved because it had the largest superconductivity R&D program of the national labs. Fitzpatrick decided that DOE should have three Pilot Centers supported by existing funds and charged with the mission of conducting cooperative R&D with industry.

What was the process for establishing the Pilot Centers?

First, DOE Secretary John Herrington and Deputy Secretary Joe Salgado requested that Los Alamos put together a plan to involve labs and industry. LANL held workshops in the fall of 1987 to provide private companies an opportunity to indicate how they would like to work with national labs on developing high-temperature superconductivity devices. In January 1988 LANL proposed the Pilot Center idea. Fitzpatrick set up an

"The organizing group identified the barriers that had to be overcome and how DOE and its contractors had to change the way we do business."

Louise Dunlap (left) and Tony Schaffhauser discuss the recent successes of ORNL's High Temperature Superconductivity Pilot Center.

internal task force within DOE to review the LANL proposal and make suggestions. From that came the suggestion that there should be three pilot centers, requiring no additions of bricks and mortar, whose sole purpose is to promote cooperative R&D agreements with industry.

LANL's proposal noted the existing barriers that make it difficult for national laboratories to work cooperatively with industry. It called for flexibility for the laboratories in negotiating agreements with industry, protection of technical data, and patent waivers. It should be noted that university contractors managing DOE facilities automatically get waivers of their patent rights under the Bayh-Dole Act, whereas industrial contractors such as Martin Marietta did not until April 1991.

A DOE task force was formed to establish and oversee the Pilot Centers. In April 1988, ORNL Acting Director Alex Zucker received a call that ORNL had been designated a Pilot Center. Bill Appleton, ORNL associate director for Physical Sciences and Advanced Materials, was assigned the job of overseeing and staffing the ORNL Pilot Center. We were named to manage the Pilot Center here. An Interlaboratory Steering Group was formed by Appleton and two associate directors at the other two labs. The DOE task force also said that the decision-making process should be delegated to the DOE Operations Offices, which had representatives on this task force. An Operations Office Steering Group was formed. They put together an Implementation Plan after the issues were discussed and resolved.

The organizing group identified the barriers that had to be overcome and how DOE and its contractors had to change the way we do business. We jointly developed issue papers, took them to Washington in August 1988, and essentially worked together to get cultural changes made in Washington. In late September 1988, Donna Fitzpatrick announced the establishment of the Pilot Centers at the World Materials Congress in Chicago. ORNL received the authorization in our portion of the appropriations bill to enter into cooperative R&D

agreements with industry. This change also required a modification of the Energy Systems prime contract with Oak Ridge Operations so that Energy Systems would have rights to intellectual property (patents) developed under cooperative agreements.

By the middle of November 1988, the Pilot Centers also obtained approval from DOE for a model agreement for use in negotiations between the Pilot Centers and private firms. This basic agreement was developed as a result of the three laboratories and three Operations Offices working together.

In short, this experimental two-year pilot program was funded for cooperative R&D and not for new bricks and mortar. We were supported by reallocated existing funds. Each pilot center was provided $1.5 million from this source for the first year. Our center started in fiscal year 1989 so the two-year term has just ended. However, our activities have been extended for two more years.

What is the purpose of the Pilot Centers?

The chief program objective is to arrange for national laboratories and private industry to conduct cooperative R&D to develop the technologies needed to accelerate the commercialization of superconducting materials and their applications. The result should make the United States more competitive with other countries in manufacturing and marketing devices using high-temperature superconducting materials.

What are the barriers to effective cooperative R&D agreements between national laboratories and industry? What progress has been made to overcome these barriers?

Before the Pilot Centers were established, there were few examples of collaborative research between ORNL and private industry. When such agreements occurred, DOE, not ORNL, negotiated the terms. The process was long and tedious; the terms and conditions with respect to ownership of data and intellectual property were fairly inflexible; and the provisions generally were onerous from industry's point of view. Then, too, the issue of augmentation of government funding with private dollars nearly always created questions and uncertainty—and sometimes killed the proposed project. As a result of these barriers, most of ORNL's interaction with the private industrial sector occurred through the well-established modes of subcontracting, work-for-others, and utilization of user facilities.

The cooperative R&D agreement, which was established for the new Pilot Centers, introduced a new dimension into the concept of government laboratories doing business with the private sector. It gave us the mechanism to put together joint ventures with industrial partners. It offered programmatic flexibility—that is, the Pilot Center projects were jointly developed and intended to be responsive to industry's needs. The cooperative agreement offered flexibility in contract terms and conditions. DOE did provide a model agreement, but within that structure there was room to negotiate. The cooperative agreement offered flexibility in funding arrangements; all projects are cost shared, but the Pilot Center can provide funding to its industrial partner to meet specific needs; the industrial partner can place funding at the Laboratory, or each party can fund its own share of the work at its own location. It offered data protection and a waiver of intellectual property rights to the inventing party—very acceptable provisions to industry. In other words, the cooperative agreement removes many barriers and allows combinations of laboratory, industry, and even university partners to get the work done in the most effective way. And, by working together in the developmental stage, the transfer of technology occurs along every step of the way—and flows both ways.

What changes have been made with respect to ownership of intellectual property developed under the Pilot Center agreements?

The question of ownership of patents developed under the Pilot Center agreements was one of the areas where private industry mandated some

"The cooperative R&D agreement introduced a new dimension into the concept of government laboratories doing business with the private sector."

When the High Temperature Superconductivity Pilot Center was established in 1988, its director was Tony Schaffhauser and its industrial partnership manager was Louise Dunlap. Since that time, organizational changes have occurred. In 1990 Dunlap became director of the Laboratory's new Office of Guest and User Interactions. Its many responsibilities include assisting the Pilot Center in developing industrial partnerships and exchanging personnel. In 1991 Schaffhauser was named associate director of ORNL's Conservation and Renewable Energy Programs. The new director of the Pilot Center, Bob Hawsey, reports to him.

changes in the way DOE normally did business. They wanted to know beforehand who would own the rights to any inventions developed under the agreement. The idea of waiting until the project was finished to ask for a waiver from DOE was not acceptable.

Industry's position could be summarized this way: "We don't like negotiating with the federal government because it takes too long and involves too much red tape. Because high-temperature superconductivity is evolving so fast, we don't have time to fool with bureaucratic procedures. If you want industry involved, the process must be expedited. Like Energy Systems, we could petition DOE for a patent waiver at the end of the project, but no waiver is guaranteed. So if we get involved in this project, we want to know who owns the intellectual property up front." Industry representatives pointed out that industry would not provide up to 50% of the funds for Pilot Center R&D unless it was guaranteed speed and simplicity in sharing the work and results and certainty in regard to who would own what and how it would be protected.

To allow the Pilot Centers to fulfill their mission, the government had to change its position. Today Energy Systems has an up-front patent waiver for Pilot Center project inventions. The ownership of intellectual property that is developed within a statement of work can be negotiated by the partners in the agreement. In other words, a private company and Energy Systems, not DOE, decide who owns the patent rights.

We jointly developed a model agreement, the starting point for all DOE Pilot Center negotiations. The areas of flexibility were defined for local approval. We worked out with the local operations office which changes they should authorize and which changes we could make if approved. Beyond that we had to go to DOE Headquarters. We worked out these areas of flexibility. We got our authorization November 15, 1988, and had our first Pilot Center agreement signed November 25, 1988, but DOE wouldn't approve it because we had made too many changes and had pushed the flexibility to the limit. This first case allowed us to determine the limits of flexibility in negotations.

This first agreement was with American Superconductor, but it took us another five months to renegotiate it so that DOE would approve it. We did start work with them in the meantime under a user agreement. The next agreement was with General Electric. GE was anxious to start work on a feasibility study of a possible invention. The company signed the model agreement as written and provided funding to ORNL for the project. So the first approved Pilot Center agreement was signed in December 1988 with GE. The people at DOE's Oak Ridge

Operations really bent over backwards. We had a tremendous working team involving our staff and people like Bob Poteat and George Manthy at ORO. It's a good example of how well ORNL and ORO can work together. Partly because of this cooperation, we were out in front of the other Pilot Centers. We had the first three agreements signed before Argonne and Los Alamos had any.

How are Pilot Center data protected?

There are two kinds of data. One type is patentable data, which are protected under our current system. We don't publish such data until a patent application for the work has been filed. If you patent something, then you have to enforce its protection. Getting a patent broadcasts that new information is available on a technology that could be useful to competitors.

The second type of data is nonpatentable intellectual property which may have near-term commercial value. Because industry is under no obligation to patent or publish the information it develops, this class of commercially valuable data is usually protected as trade secrets. When a company shares such information with us, we treat it as proprietary information as long as it is not patented or published.

However, data developed within the scope of Pilot Center agreements are not proprietary because the government has supplied 50% or more of the funds for the development. So a third class of data, called "limited access" data, which can be protected for two years, was defined. Under an agreement, the company has access to our data and we have access to theirs. The government can have access to it for national security reasons. Once data have been stamped "limited access," the company's competitors cannot have access to them, and because they are not yet government-owned data, they are not accessible under the Freedom of Information Act. At the end of the two-year protection period for limited access data, they revert to government ownership and are available to the public. This arrangement gives the industrial partner a head start because part of the initial R&D cost was paid by the government.

With all the restrictions on data publication, will ORNL researchers get proper credit for their research on Pilot Center projects? What happens to patents?

The basic research data that come out of the Pilot Center are made available to the technical community and are published if the participants agree. We don't throw a blanket over all the data. It's only in the case of key trade secrets that we do not want to give away the store. We have a lot of good scientific publications coming out of our Pilot Center. In general, industry wants to publish the good scientific data, and, of course, our people need to publish.

As to class-waiver patent rights, industry owns all the patents developed by their employees within the scope of the cooperative agreement. The federal government retains a royalty-free license for government purposes because the government is cost sharing. There is also a waiver of patent rights by DOE to Energy Systems. We can give our industrial partners preferred licensing terms. It depends on who is bringing what to the table. Because Energy Systems has the ownership of patent rights, we can cross-license the technology to our industrial partners. The patent must be assigned to one organization or the other even though persons from both organizations can be listed on the patent. In most cases, a patent is an asset to the company.

The decision on which organization the patent is assigned to is made on the basis of what will be in the best interest of commercialization. In general, an industrial firm is given the patent rights to facilitate commercialization. However, that was not true in the case of our cooperative agreement involving Bellcore, which is the old research arm for the Bell operating companies. When AT&T was split up and put under antitrust supervision, Bellcore could not give an exclusive license to anyone. Bellcore asked Energy Systems to keep the patent and asked for an exclusive license only for the field of use. Bellcore told Energy Systems, "You are free to license it elsewhere and we will share the royalties. Sometimes a small company

"Today Energy Systems has an up-front patent waiver for Pilot Center project inventions."

"We get approval of a model Pilot Center agreement in two weeks or less."

prefers that Energy Systems has the patent because, as a large company with its own lawyers, Energy Systems may be in a better position to enforce the patent than a small industrial partner. It's a negotiable matter. The decision is based on what's good for commercialization and ultimately for the competitiveness of the nation.

Will the Pilot Centers take advantage of cooperative research and development agreements (CRADAs), the new provisions for industry-government research?

Actually, the successful operation of the DOE Pilot Centers provided the model for the concept of CRADAs. CRADAs have some advantages over the cooperative R&D agreements we now sign; for instance, they offer better data protection. ORNL was one of the first laboratories to be authorized to enter into CRADAs because Energy Systems and DOE negotiated the required contract change. The first CRADA was signed with the international industrial consortium called the Alternative Fluorocarbons Environmental Acceptability Study (see "Technology Transfer" in this issue for details).

A CRADA does not allow transfer of funds to industry as a Pilot Center R&D agreement can. A separate subcontract is required, and the approval process for a CRADA is more formal and drawn out for up to 90 days. We get approval of a model Pilot Center agreement in two weeks or less.

What kinds of companies is the Pilot Center working with?

We are working in several technical areas with industry, and we have signed agreements with a good mix of large and small companies. We are conducting cooperative research with large companies like Corning, DuPont, General Electric, IBM, and Westinghouse Electric, and with small startup companies like American Superconductor; Superconductivity, Inc.; HiTc Superconco; Consultec Scientific; and American Magnetics. The last two companies are local. Other companies are IMTech, CPS Superconductor, Dow Corning, Textron Specialty Materials, and EMCORE.

Any major achievements so far?

We have fabricated some superconducting wire under a cooperative agreement with American Superconductor. American Superconductor provided ORNL with feed material called BSCCO because it is made of bismuth, strontium, calcium, and copper oxide, using a previously developed proprietary process. A group led by ORNL principal investigator Vinod Sikka fabricated the wire from the feed material, and American Superconductor heat treated the wire to give it optimum superconducting properties. Then we both characterized the treated wire and measured its superconducting properties (see photograph on p. 9). The company sent one of its employees to work with us part time. ORNL and American Superconductor exchange information and ideas by a weekly fax report and a biweekly conference call.

Corning developed a flexible ceramic substrate made of fully crystallized, partially stabilized zirconia. It is not ductile, but it is very thin and tough like fiberglass. Corning did not have the ability to deposit a good superconducting material on this substrate, but we were able to deposit a YBCO (yttrium barium copper oxide) material on it using laser ablation. We had tried laser deposition before, but we used other, less effective substrates. This was a mutually beneficial joint venture—we had something they needed and they had something we needed, a good proprietary substrate. Both parties brought something to the table. Together we have developed a superconducting tape that could be used for winding a magnet. Also, because the zirconia absorbs little microwave energy, the tapes could be used in microwave oscillators for communications between satellites.

We have also developed a new design for a superconducting motor. We are building superlattices in which conducting layers of YBCO material only a few atoms thick are sandwiched between insulating layers of magnesium oxide;

Ken Blakely, ORNL technician, checks the flexibility of 60 ft of superconducting BSCCO wire made under a cooperative agreement between ORNL/Energy Systems and American Superconductor, Inc.

Amit Goyal inserts a sample of a high-temperature superconducting material into the cryostat used to measure the properties of a superconducting wire sample in the liquid-helium to liquid-nitrogen temperature range. He is working with Don Kroeger of ORNL's Metals and Ceramics Division under collaborative research agreements with American Superconductor, General Electric, and Westinghouse.

ORGANIZATION	TECHNOLOGY AREA
Advanced Fuel Research	In situ deposition monitors
American Magnetics/Georgia Tech	Characterization of chemical-vapor–deposited multifilament conductors
American Superconductor	Fabrication of wire and tape
Astronautics	Magnetic heat pumps
Consultec Scientific	Deposition target device
Corning	Deposition on flexible ceramic substrates
CPS Superconductor	Melt processing filaments
Dow Corning	Thick film deposition
DuPont	Thin-film devices and bulk applications
Electric Power Research Institute (EPRI)*	Superconducting motor testing and power electronics
Energy Conversion Devices	Laser deposition of conducting materials
General Electric	Thallium superconducting material processing
HiTc Superconco	Magnetic bearings
IBM/Ames Lab	Optimized flux pinning
Intermagnetics General Corp. (IGC)*	Optimized flux pinning
Innovative Materials Technology	Composite tape fabrication
Neocera	Thin film deposition
Reliance Electric*	Magnet testing for motors
SUNY-Buffalo	Laser deposition of conductors
EMCORE/Stevens/Rutgers	Chemical vapor deposition for electronic devices
Superconductivity, Inc.	Magnetic energy storage for small systems
Textron Specialty Materials	Deposition of conductors
Westinghouse Electric/ Univ. of New Mexico	Powder scale-up and wire fabrication

* Pending cooperative agreement.

ORNL's High Temperature Superconductivity Pilot Center has signed 20 cooperative R&D agreements with private companies and other organizations, and three more agreements were pending in June 1991.

these could be used for switching devices. And we are making excellent superconducting thin films.

We are learning about the enhanced ability of BSCCO to carry large currents. When melted in a silver tube, BSCCO offers excellent superconducting properties at temperatures higher than the boiling point of liquid helium (4.2 K) but lower than the boiling point of liquid nitrogen (77 K). Today, thin YBCO superconducting films are as good at 77 K as Nb_3Sn is at 4.2 K. However, bulk YBCO materials are far off the mark at 77 K, even though they may be acceptable at 20 K.

Does the Pilot Center take advantage of ORNL's user facilities and great capacity for interdisciplinary research?

Definitely. ORNL's superconductivity researchers include physicists, chemists, metallurgists, mathematicians, and engineers. They come from the Applied Technology, Chemistry, Engineering Physics and Mathematics, Fusion Energy, Metals and Ceramics, and Solid State divisions.

The only user facility used extensively so far is the High Temperature Materials Laboratory. Some superconductivity research has been done at the Shared Research Equipment facility and the Surface Modification and Characterization Collaborative Research Laboratory. Now that the High Flux Isotope Reactor is operating reliably, work on characterizing high-temperature superconducting materials is being done at the HFIR's Neutron Scattering Facility and National Center for Small-Angle Scattering Research.

What has been the Pilot Center's chief contribution to the progress made in getting high-temperature superconducting materials out of the laboratory and into the marketplace?

The bottom line is that the Pilot Centers provide industry easier access to national laboratory resources and technology. This joint venture approach allows industry-driven applications and development that should expedite commercialization. Intellectual property rights are now protected for the benefit of U.S. industry. The Pilot Center concept, which has been declared a success by DOE, provided the model for implementation of CRADAs as described in the 1989 amendment to the Stevenson-Wydler Act.

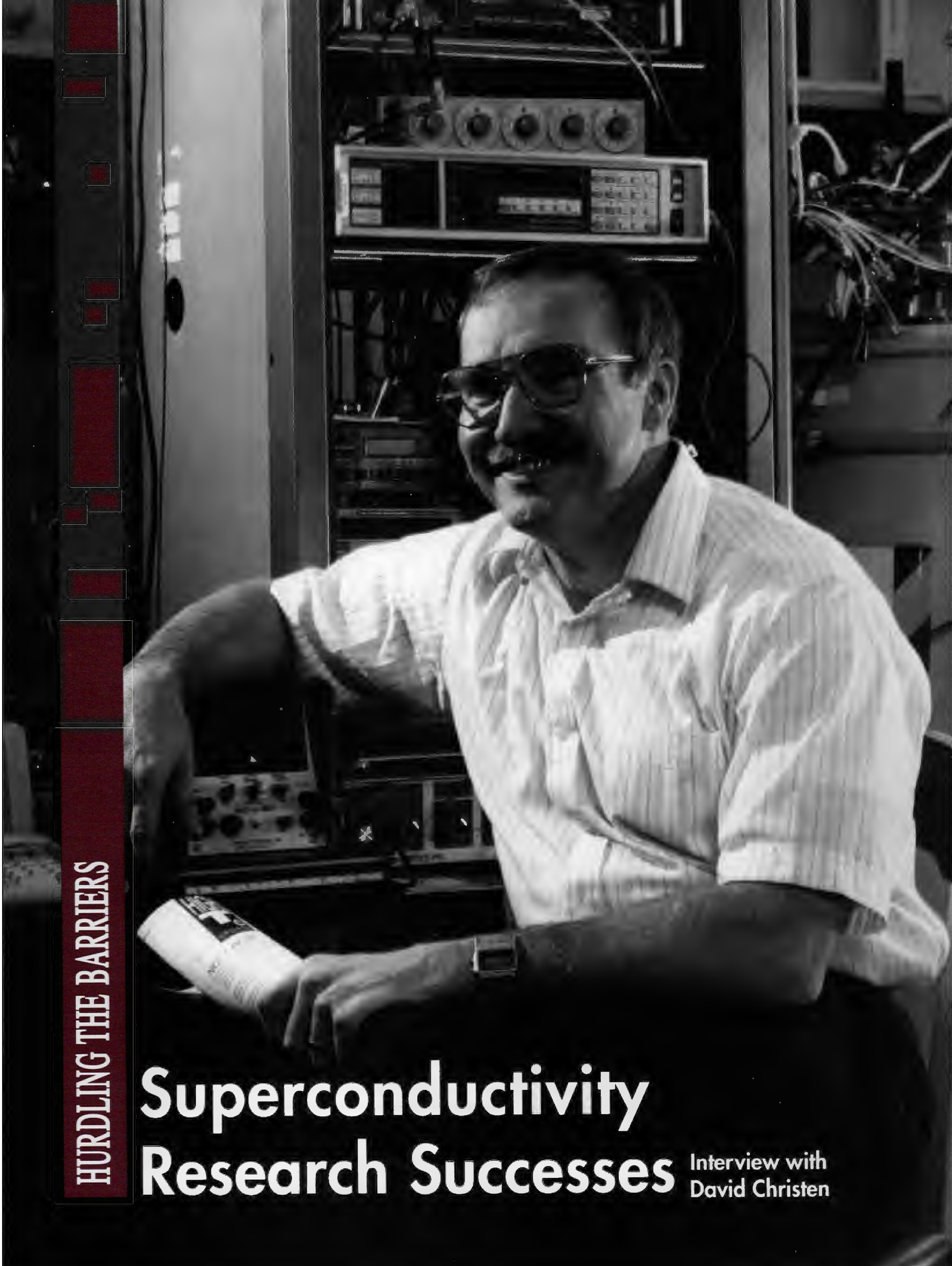
"The bottom line is that the Pilot Centers provide industry easier access to national laboratory resources and technology."

What is the future of the Pilot Center?

The Pilot Center has a promising future. As a result of its success in working with industry, the Pilot Center has received increased funding, from $1.9 million last fiscal year to $3.5 million this fiscal year. We think that our work at ORNL in cooperation with our industrial partners will help put the developments of the laboratory into the hands of consumers in a very short time. The Pilot Centers have helped overcome the technical and institutional barriers of developing and transferring the technologies that are emerging as a result of the discovery of high-temperature superconductivity five years ago. ornl

For more information, call Tony Schaffhauser at 615-574-4826.

HURDLING THE BARRIERS



Superconductivity Research Successes

Interview with David Christen

David Christen, sitting in front of ORNL's Critical Current Density Cryostat, is pleased with the latest results from experiments on superconducting films to determine the effects of defects on their magnetic flux pinning and ability to carry current.

About four years ago, scientists discovered materials capable of conducting electricity with zero resistance when chilled by liquid nitrogen. The discovery of these high-temperature superconducting materials caused a stir because liquid nitrogen and refrigeration in the liquid nitrogen temperature range are much less expensive than liquid helium, which is used to cool conventional superconductors. Thus, if these materials could be used to make practical, low-cost, energy-saving superconducting devices, the electrical world would be revolutionized. The news media proclaimed that the discovery could lead to high-speed computers; long-distance power transmission; more efficient medical diagnostic devices; and high-speed, levitated trains.

Scientists from Department of Energy laboratories, including ORNL, joined the frantic effort to advance the technology by striving to achieve several new goals: (1) fabricate flexible wires and films from high-temperature superconducting materials, which are largely brittle ceramics; (2) increase the current-carrying capacities of these materials so they can conduct usable amounts of electricity in a magnetic field; (3) develop new low-cost, energy-saving superconducting devices; and (4) arrive at a theory to explain high-temperature superconductivity.

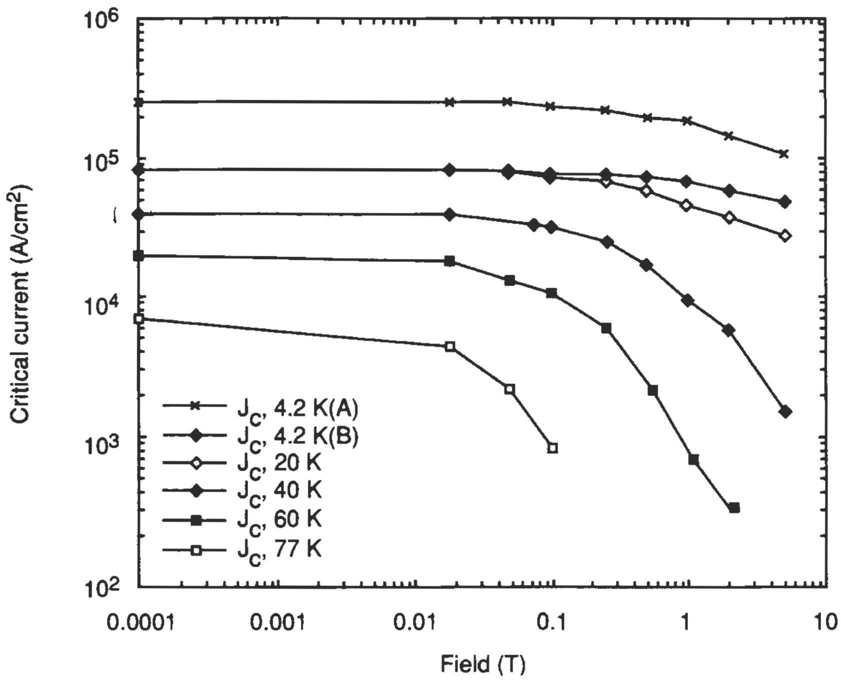
How close have U.S. scientists in general and ORNL scientists in particular come to achieving these new goals? How does our progress compare with that of the Japanese and Europeans? To answer these questions, the *Review* staff interviewed David Christen, scientific coordinator of the High Temperature Superconductivity Pilot Center at ORNL.

In 1987, several goals were set following the discovery of high-temperature superconductivity. Since then, a number of advances have been made, but barriers still remain. What progress has been made with respect to the goal of turning brittle superconducting ceramics into flexible wires and films?

In 1989 scientists made a quantum leap in progress. We can now make flexible cables from superconducting materials potentially capable of conducting large currents in large magnetic fields. Advances have occurred as the result of a discovery by the German company Vakuum-Schmelze that enhanced current conduction is obtained from bismuth-based superconductors melted inside silver tubes. The compound used is called BSCCO because it contains bismuth, strontium, calcium, copper, and oxygen. It has since been found that superconducting tapes that conduct large currents can be formed by packing powders of these bismuth-based materials in silver tubes, drawing the tubes into wires, and flattening them into tapes. By melting the materials inside the tapes, a nice stack of superconducting, crystalline plates is formed that conducts current in a desirable direction along the copper-oxide basal planes down the length of the cable.

The key to superconducting tapes and flexible cables is good material preparation. It's quite empirical. The Japanese have taken the lead, but two or three U.S. companies and laboratories are at the forefront as well, and ORNL is one of them. The companies we have been collaborating with through a High Temperature Superconductivity Pilot Center agreement, American Superconductor

Amit Goyal, a Ph.D. candidate from the University of Rochester, uses ORNL's electron microprobe system shown here to determine the varying compositions (phase content) and phase distribution in a metal-processed YBCO sample.



A DOE-EPRI assessment of high-temperature superconductors shows the estimated target values for critical current density and magnetic field strength for YBCO, BSCCO, and Nb_3Sn for several applications.

Corporation of Boston and Westinghouse Research Laboratories, had been working on the yttrium-barium-copper-oxide (YBCO) material, but as soon as the company heard about the German work, it started developing BSCCO and duplicated the German results. The Japanese have been working with bismuth-based materials all along because they first discovered that BSCCO materials can achieve high-temperature superconductivity.

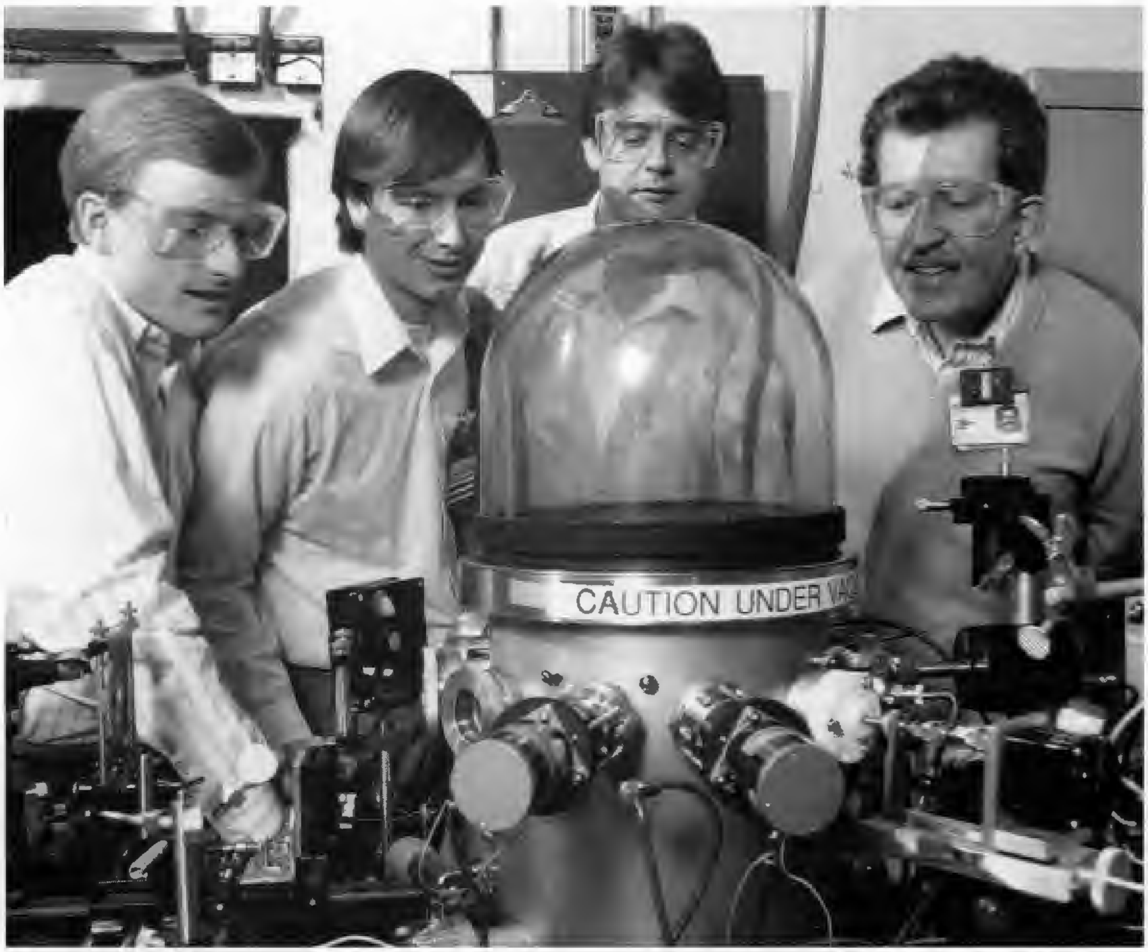
This powder-in-tube melt processing does not work as well for YBCO as it does for BSCCO. Its anisotropic variations are not as large—that is, the differences in superconducting properties along different crystal directions are smaller than those in the bismuth materials. The YBCO crystals don't grow as rapidly in the copper-oxide basal planes as the bismuth does. The other problem is that YBCO cannot be melted in the silver tubes because its melting temperature exceeds that of silver. Silver is needed because it acts like a catalyst, enhancing crystal growth. In addition, silver is a relatively inert metal and acts as a stabilizer that, in proximity with the bismuth, provides an alternate current shunt in case the superconductor becomes normal.

The problem is that, unlike YBCO, BSCCO appears to have an intrinsic problem with conducting currents at high temperatures—say above 30 or 40 K. YBCO has these problems less severely; it is more attractive at liquid nitrogen temperatures.

Right now, scientists are focusing on developing bismuth-based cables that would operate not at liquid-nitrogen temperatures (77 K) but in the liquid-hydrogen (20 K) or liquid-helium (4.2 K) range. BSCCO has an advantage over conventional low-temperature superconductors, such as those containing niobium-tin or niobium-titanium: it can sustain much higher magnetic fields in liquid helium—more than 30 tesla (T) rather than just 20 T. In the near term, these materials could be used to make hybrid helium-cooled superconducting magnets in which the outer part of the superconducting solenoid would consist of conventional superconductors and the inner part, which is designed to sustain a really high field, would contain bismuth-based materials.

But isn't the cost of liquid helium a deterrent to fabricating low-temperature superconducting magnets?

It's true that liquid helium is 15 times more expensive than liquid nitrogen. That's why some high-temperature superconductor applications are attractive. Liquid helium costs $3/L and liquid



Examining the Solid State Division's pulsed laser-ablation system for depositing high-temperature superconducting films onto a proprietary flexible ceramic substrate developed by Corning are, from left, Willard Cutler and Dell St. Julian, both of Corning, Inc., and David Norton and Doug Lowndes, both in the Solid State Division.

nitrogen costs about $0.20/L. But helium is abundant in the United States because it occurs in certain natural gas deposits. In Europe, helium is more expensive because it must be distilled out of the air. Anyway, it turns out that for many large-scale applications, the operating costs are trivial compared with the capital investment.

Is ORNL making superconducting films of value to industry?

ORNL is working with three companies on superconducting films and deposited tapes through cooperative R&D agreements made through the Pilot Center. An ORNL group led by Doug Lowndes and Dave Norton, both of ORNL's Solid State Division, is using laser ablation to deposit superconducting YBCO films on polycrystalline zirconia tapes made by Corning. The 20-µ-thick tapes are tough and flexible; they can be wrapped around a finger without breaking. We are working together to determine the highest-quality superconducting film that can be put on such a tape and how this might be scaled to a continuous process. The superconducting tapes might be used to wind magnets or other types of conductor devices.

University of Tennessee graduate student Shen Zhu inspects the system for pulsed laser deposition of thin films of high-temperature superconducting material.

In another Pilot Center agreement with DuPont, Lowndes and Norton are depositing high-quality, epitaxial films on large-area substrates of single-crystal magnesium oxide. DuPont supplies the substrate and is attempting to develop the films for various microwave applications.

The properties of materials such as superconductors cannot be properly studied unless good processes are used to make uniformly high-quality samples. Yurolf Brynestad of the Chemistry Division has worked to develop thick and thin thallium films for use by the General Electric Company in another Pilot Center cooperative agreement. Brynestad is the only superconductivity researcher at ORNL with the appropriate equipment to work with such a toxic material as thallium. He makes precursor materials and reacts them with thallium vapor to form a superconducting compound. After the material is subjected to final heat treatment in a well-controlled environment, thallium films are formed for research by GE. Thicker deposits of melt-processed YBCO and BSCCO on metal substrates are being developed for conductor applications by Don Kroeger, Fred List, and Amit Goyal.

What progress have scientists made in increasing the current-carrying capacities (critical current density) of the new high-temperature superconducting materials? Have they reached the goal of increasing it by a factor of 100?

The ability of a superconductor to carry a loss-free direct current is limited by the so-called critical current density J_c. The critical current density of a superconductor depends sensitively on the material's microstructure.

The J_c of these new materials has been increased considerably by altering the crystal, or grain, alignment to improve current flow in the copper oxide basal planes. By aligning all the grains preferentially, scientists have increased the critical current density by a factor of 100 since 1987. Of course, this factor varies with ranges of temperature and magnetic field strengths.

ORNL scientists conducted research to help overcome the barrier of low current density. Don Kroeger and his colleagues in our Metals and Ceramics Division set out to determine why grain boundaries—contact areas between crystals similar to the cement between bricks in a wall—are barriers to current conduction. They looked at the question from a bulk materials point of view. Lowndes and Norton looked at the same question from a thin-film materials point of view, providing complementary information. Kroeger investigated the chemical makeup of the grain boundaries. He tried to find out if the chemistry of these materials at the grain boundaries caused a barrier to the conduction of current. Two factors were found to be important: chemistry and the huge anisotropy in crystal growth and electronic properties.

In the thin film work, the scientists deposited films on polycrystalline rather than single-crystal substrates and observed that, although the grains had a common crystal axis perpendicular to the substrate surface, they had a random orientiation in the plane of the substrate. They observed that, if the grains are not aligned in-plane or do not match up at specific grain-boundary angles, the current-carrying capacity is reduced.

Corning made this polycrystalline zirconia tape, which is coated with one of ORNL's superconducting films. The superconducting tape is still fairly flexible.

Current flows through a bulk material in a different way than through a thin film. Because the grain boundaries of films pass all the way through vertically from the substrate to the surface, the current must run straight through the grain boundaries. In the bulk materials, such as the melt-processed bismuth-based superconductors, the crystal plates overlap as in a brick wall. When the current reaches a grain boundary in the base, it sees a weak link but a huge cross-sectional area through which it can transfer up to another grain and then conduct along that grain. In the brick wall analogy, instead of going through the cement from one brick horizontally to another, it goes from one brick to the overlapping brick above and down to the next brick. In other words, the current zigzags through the bulk rather than going straight, as in film.

Kroeger and his colleagues found that, if the aspect ratio of the crystal plates is very long and very thin, then the overall current density can be quite high. In other words, the longer and thinner the plates (bricks), the better the current transfer. The bulk BSCCO material can carry more current than a YBCO film on a polycrystalline substrate but not nearly as much as a YBCO film on a single-crystal substrate. Kroeger and collaborators are determining whether the chemistry, aspect ratio, or structural characteristics make bismuth materials able to carry more current than polycrystalline YBCO films.

Jorge Ossandon (left), on leave from the University of Talca, Chile, and Dave Christen of ORNL's Solid State Division use the SQUID magnetometer to measure magnetic flux pinning and other magnetic properties in superconducting materials having various defects. In the background is vapor from liquid helium used to cool the SQUID magnetometer.

In work that my group has been involved in with IBM's Thomas Watson Center, we have used proton irradiation to introduce controlled defects into well-characterized YBCO crystals in order to pin the magnetic flux lines. Our goal is to alter superconducting materials to optimize flux pinning and get the maximum current-carrying capacity at high temperatures and high magnetic fields. We have already introduced damage in single crystals to increase current-carrying values to levels close to those of epitaxial thin films.

Are scientists and engineers on the brink of developing new superconducting devices?

Superconducting devices are on the way. Superconducting Technologies, Inc., in California is now preparing to sell thallium thin-film microwave filters and strip lines. The deposition of superconducting films on substrates can now be controlled well enough to produce uniform, high-quality products. Superconducting microwave filters are superior to copper, gold, or silver filters for microwave transmission devices for satellite communications because they conduct microwaves with minimal losses, which greatly sharpens the filter response.

I think the first widespread use of novel superconducting materials will be for cables, which will probably be used initially for conducting current into existing high-field superconducting magnets; copper wire is not good for this purpose because of its resistive losses and large heat conductance, which consumes power and boils away the refrigerant. The potential applications are magnetic energy storage, power transmission, and superconducting motors and generators.

The second wave of devices will be passive electronic devices made from superconducting films. These would include microwave filters and superconducting interconnects. ORNL and other organizations have made great progress in developing high-quality, virtually single-crystal thin films that can be deposited on appropriate substrate materials. Through the science of epitaxy, scientists have learned how to match the registry of atoms in a superconducting film with the registry of atoms in the single-crystal substrate on which the film is deposited. Single-crystal superconductors consisting of YBCO or thallium-based films have

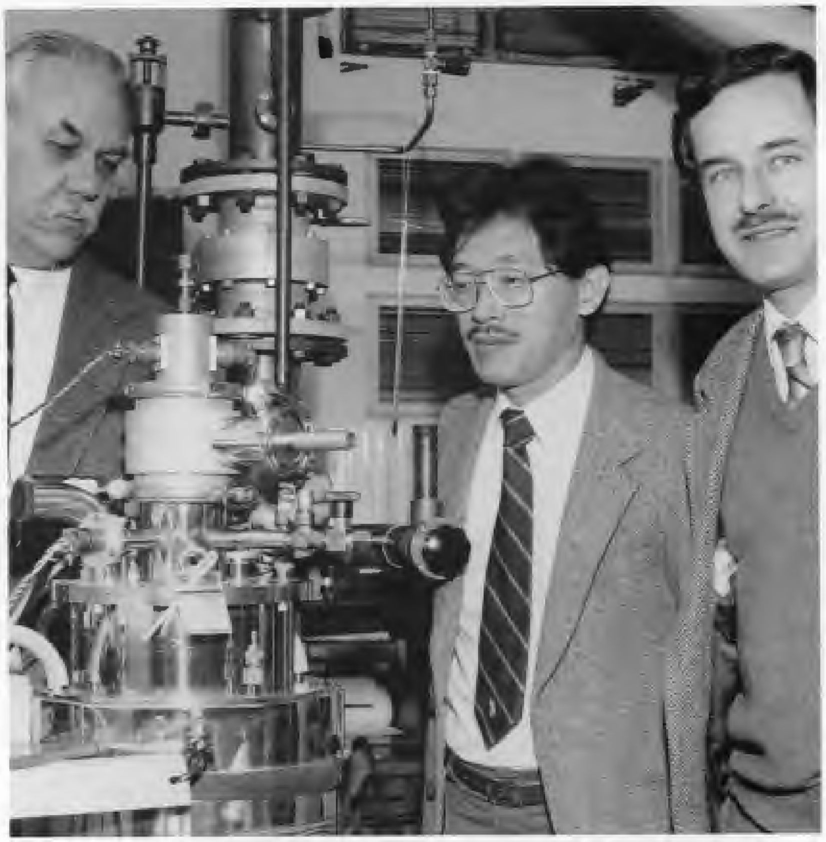
Physicist Winston Chen (right) of ORNL's Health and Safety Research Division performs collaborative research on superconductivity with three representatives of Advanced Fuel Research, Inc., in East Hartford, Connecticut—from left, David Fenner, Phillip Morrison, and John Haigas. They are using a Fourier-transform infrared spectroscopy system built by Advanced Fuel Research and installed at ORNL. It will be used for in situ diagnostics during laser ablation to ensure optimal deposition of superconducting thin films.

excellent properties for filters for transmitting microwaves at specific frequencies with virtually no energy losses.

Another application for thin films is in superconducting interconnects for carrying current in the next generation of supercomputers. These films take less space and dissipate much less power than the conventional copper wire interconnects. To increase computer speed, the circuits must be packed ever more tightly to shorten the distance that electrical signals travel. For the achievable limits of so-called "multichip modules," superconducting films are essential as interconnects between integrated circuits because, unlike thin copper wires, they emit no potentially circuit-damaging heat.

I predict that the third generation of superconducting devices will be active electronic devices such as light-sensitive and infrared detectors based on superlattices. ORNL has been at the forefront of the construction of these artificially structured multilayers of thin films. A superlattice consists of an epitaxial structure in which a series of superconducting and insulating layers several atoms thick are sandwiched together, making the distance between these layers very small. These superlattices may offer totally unique properties and the potential for new applications. Doug Lowndes, Dave Norton, and Dave Gohegan, all of ORNL's Solid State Division, have made superlattices from layers of YBCO sandwiched between insulating layers of the rare earth praesodymium-BCO.

"ORNL and other organizations have made great progress in developing high-quality, virtually single-crystal thin films that can be deposited on appropriate substrate materials."



Don Kroeger (left) of ORNL's Metals and Ceramics Division; Huey Hsu, former ORNL researcher and a consultant to American Superconductor; and Alex Malozemoff, vice president for research and development at American Superconductor, examine a cryostat (made by American Magnetics of Oak Ridge) for measuring current density in superconducting materials.

High-temperature superconductors may also be used as active switching devices because these materials are so anisotropic. Because their superconducting properties are different along one crystal direction from those in another crystal direction, a very fast "on" and "off" switch may be possible.

What about superconducting motors, such as the prototype recently developed at ORNL?

The next important use of high-temperature superconductors will be for generators and electric motors. As you have noted, an important step in that direction has already been made at ORNL.

In collaboration with the Electric Power Research Institute and with internal financial support, ORNL has designed and developed a new prototype superconducting motor constructed from magnets wound with conventional superconducting materials made of niobium and titanium. These stationary magnets produce a rotational motion by interacting with a radial current flowing in two rotating armature assemblies, one on each side of the stationary cryostat. The new motor design allows the conventional superconducting magnets to be replaced with high-temperature superconducting magnets as soon as the appropriate wires and compact refrigeration system are available. The new motor began operating on September 21, 1990 (for more details, see sidebar on p. 24).

What progress has been made in developing a theory to explain why some materials are superconductive at temperatures above 23 K?

The fundamental mechanism for high T_c is still not understood. T_c is the critical temperature at which a material abruptly loses its resistance to the flow of electricity. High T_c may be defined as the temperature exceeding that of the best "conventional" superconductor—about 23 K.

Several alternative models of high-T_c mechanisms have been proposed, and those models are being tested. No definitive answer has emerged.

At ORNL Malcolm Stocks, Sam Liu, Richard Klemm (visiting scientist, now at Argonne National Laboratory), Dick Wood, Mark Rasolt, and Mark Mosteller have done theoretical work on the fundamental pairing mechanism. It is fairly evident that superconductivity occurs because the conduction electrons form pairs, which move in step with each other, rather than collide with each other and dissipate heat, as do the electrons in normal resistive conductors. Liu and Klemm developed a new model to address this question: If a pairing mechanism exists, how does it manifest itself in highly anisotropic crystalline layers found in high-temperature superconductors?

Stocks, who is with the Metals and Ceramics Division, has been working with Al Geist of the Engineering Physics and Mathematics Division to use the new Intel parallel computer to do high-speed simultaneous calculations of the electronic structure of YBCO materials. Also in the M&C Division, Bill Butler and Nancy Wright have developed an ionic model for the structural stability of YBCO superconductors.

In the Solid State Division, Wood and Rasolt have independently done some nice work in interpreting how T_c is influenced by the relative thicknesses of conducting and insulating layers in superlattices. When a superconductor and an insulating layer are in proximity, experiments show that varying their relative thicknesses changes the T_c. Why? Wood's explanation has to do with the transfer of electronic charge carriers from the praesodymium insulating layers to the YBCO conducting layers, and Rasolt's interpretation is based on two-dimensional electronic effects arising from the very thin layers.

The High Flux Isotope Reactor was not operating in 1987 when high-temperature superconducting materials were discovered. But now it is back in operation. How will neutron scattering research at the HFIR aid our understanding of these materials?

Of course, neutron scattering is a very powerful tool for the study of materials in general. Both the wavelength and the energy of neutrons are well-matched to interatomic spacings and excitational energies in solids, and the neutrons penetrate all the way through large samples. By using small-angle neutron scattering, researchers can measure the relatively large spacings between the quantized magnetic vortices, thus obtaining a real microscopic picture of a vortex lattice. Recent measurements at the HFIR by Herb Mook of the Solid State Division show that the vortex structure in a unique, cubic oxide superconductor is dependent on temperature and magnetic field. Also, Mook has recently used inelastic neutron scattering to measure the Doppler shift associated with atomic vibrations in the YBCO and BSCCO high-T_c materials. He has found a significant shift in the in-plane copper atom vibrations as the sample is cooled through the superconducting transition temperature. This result is important because it implies that lattice vibrations provide the mediating attractive interaction between electrons that is responsible for superconductivity. It was previously thought that this mechanism was too weak for high-T_c superconductivity, although there is clear evidence for electron-lattice interactions in conventional superconductors.

In terms of the science and technology of superconductivity, is the United States competitive with the rest of the world? In what ways is Japan ahead of the United States? Are any other countries ahead of us? If so, in what ways?

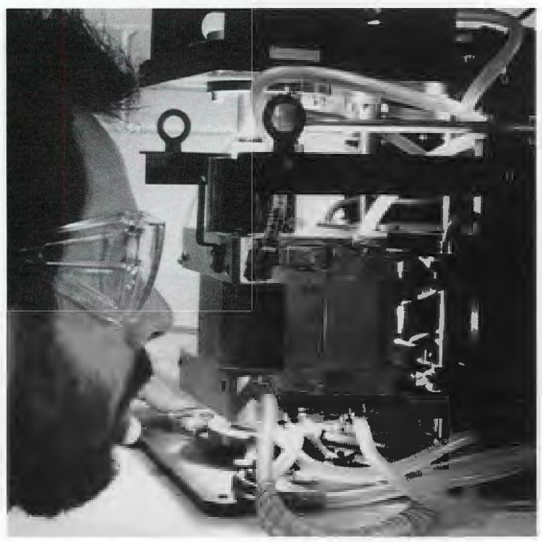
The United States is competitive. We are leading the world in the fundamental understanding of superconducting properties. From attending international conferences, my reading is that the Japanese are ahead of us in fabricating flexible cables, but they lag behind us in the fundamental sciences. They seem willing to let the United States do the basic science, while they apply the findings—a familiar scenario! I think the Europeans are doing well in basic science and, in isolated cases, in applications.

Vakuum-Schmelze, which discovered the enhanced conductivity of bismuth-based materials melted in silver tubes, and Siemens, another German company, are doing excellent development work.

What does ORNL need in terms of funding, equipment, and personnel to be competitive with other national laboratories and labs in other countries? Does industrial cooperation help make up for any deficiencies here?

We were equipment rich and personnel poor in 1987, and now we are pressed in both areas as a result of expanded efforts. When we take on a collaborative investigation with a private company through the Pilot Center, we get financial support to bolster personnel. But we have found that we are now equipment limited. Until recently no mechanism existed to handle that. But the Pilot Center is getting its first capital equipment budget to remedy this problem.

As for the base programs for superconductivity research at the national laboratories, ORNL has one of the smaller efforts. Thanks to these efforts and Pilot Center industrial cooperation, the Laboratory has stood out in terms of what has been accomplished per dollar invested in superconductivity research. Industrial cooperation gives us an opportunity to be relevant, to find applications for high-temperature superconductivity by taking advantage of our basic expertise in materials fabrication and characterization.



Bryan Chakoumakos inspects a high-temperature furnace for growing single crystals of superconducting oxides.

What are ORNL's strengths in respect to understanding and finding applications for high-temperature superconducting materials?

One strength is our ability to make high-quality superconducting thin films and deposit them on a variety of substrates. Doug Lowndes, Dave Norton, Doug Mashburn, and Ron Feenstra have done some excellent work in understanding why high-quality films are such good current conductors. Recently, John Budai, Feenstra, and Terry Lindemer have studied very systematically the effects of thermal processing on the structure and superconducting properties of YBCO films. Their results will have a major impact on the field.

Another strength is our ability to synthesize high-quality superconducting materials. Lynn Boatner, Brian Sales, and Bryan Chakoumakos, all of the Solid State Division, are growing single crystals to understand the basic properties of superconducting materials. The strongly anisotropic properties of these materials can only be understood by studying them in single-crystal rather than in polycrystalline form. In addition, highly homogeneous submicron powders are prepared by Huey Hsu (consultant from IMTECH) and Don Kroeger using an aerosol pyrolysis technique. These starting materials are used in a promising approach to conductor fabrication that involves melt-processing of thick powder deposits on metallic tapes. This approach may overcome the existing grain-boundary problems that currently prevent YBCO, with its superior intrinsic properties, from being exploited in conductor form.

The Laboratory's extensive materials fabrication capabilities, directed by Vinod Sikka of the M&C Division, have been an important element in our collaborative effort with American Superconductor Corporation to develop practical conductors using BSCCO. Also significant is our ability to study the important effects of grain boundaries and intergrowths on critical current density in all these materials with an aim toward conductor applications. Kroeger, Bob Williams, and Fred List, all in the Metals and Ceramics Division, and postdoctoral fellow Amit Goyal work on this project.

We also have a strong capability in studying the microstructure of various superconducting materials and in relating it to actual properties. Steve Pennycook, Matt Chisholm, and John Budai, all of the Solid State Division, and Kathy Alexander of the M&C Division have been studying microstructural properties. Budai uses X-ray diffraction, and Pennycook uses his own Z-contrast technique to achieve chemical sensitivity at atomic resolution in a scanning transmission electron microscope. They are trying to determine why some materials are better superconductors than others by comparing grain alignments as well as defects, second phase intergrowth, and atomic spacings in the crystal lattices.

Another strength is our ability to determine and measure the fundamental properties of materials, including superconducting properties. One basic property that I am studying, along with my Solid State Division colleagues Jim Thompson, Rich Kerchner, Charlie Klabunde, and our graduate students, is flux pinning. Our group is also working with IBM on flux pinning through a Pilot Center cooperative agreement.

In this work, we systematically introduce defect structures into single crystals and thin films of YBCO and study flux pinning, flux motion, and magnetic relaxation. By introducing defects in a controlled way using proton and heavy-ion accelerators, we have raised J_c flowing in the copper-oxygen planes by a factor of 100. This irradiation technique is not practical for a general application, but it may help guide us to, say, a metallurgical process that introduces desirable defects during material fabrication.

In high magnetic fields, J_c is limited even in the best epitaxial films. In studying the limits to J_c, we find that, under certain conditions, these materials can conduct very high currents almost intrinsically if the superconductor's external magnetic field is oriented parallel to the copper-oxygen planes. In this case, the YBCO material can conduct at 77 K as large a J_c as niobium-tin (Nb_3Sn) at 4.2 K. But the materials are highly anisotropic, and if rotated to the other orientation, they perform less favorably because of weaker pinning and thermally activated flux motion.

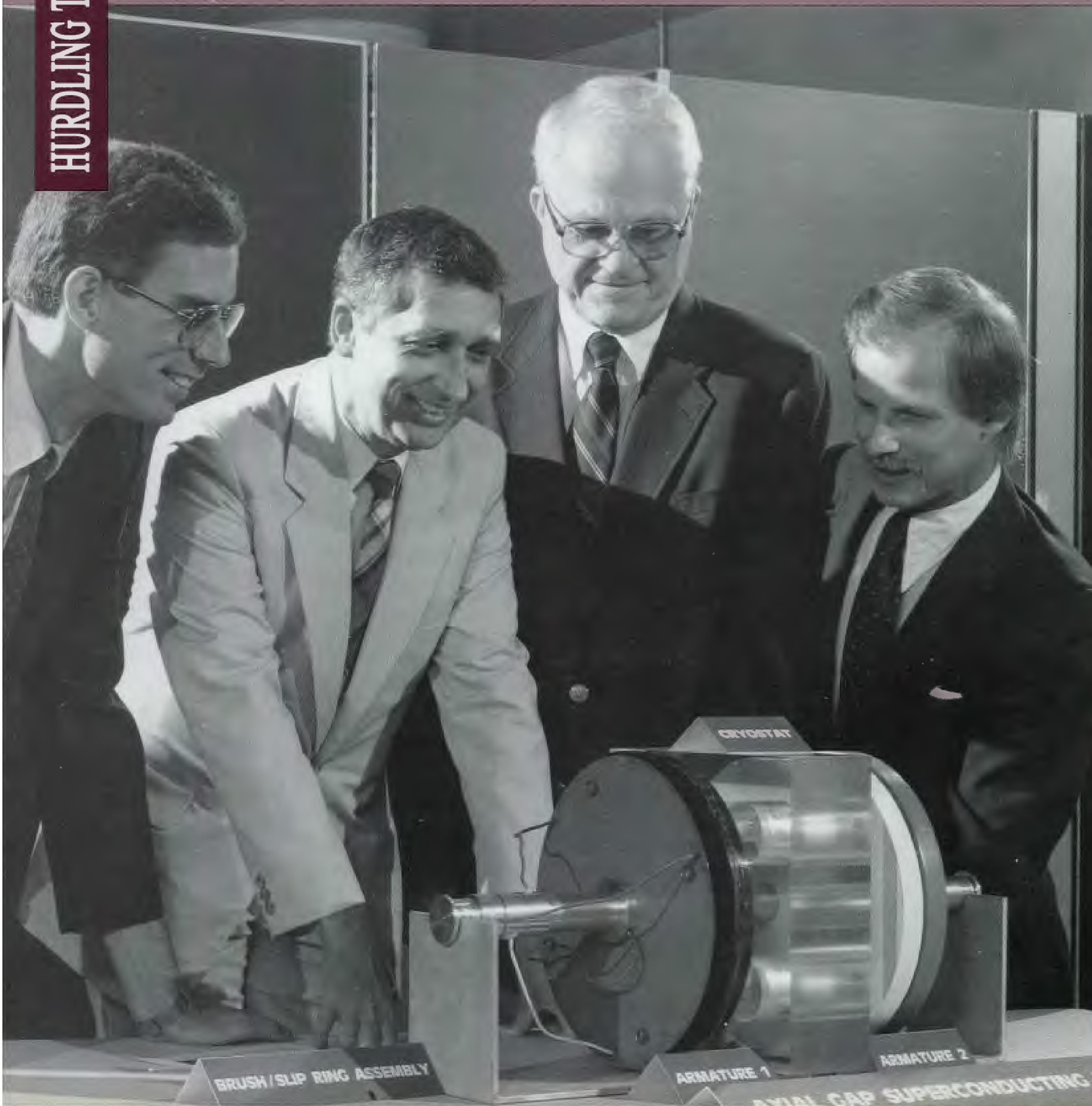
How can magnetic flux pinning help?

Magnetic flux pinning refers to the ability of the microstructural defects in the crystal lattice to prevent motion of the quantized magnetic flux lines. Flux lines are entities that occur naturally as part of the magnetic structure of a superconductor when it is in a large magnetic field. For a perfect superconductor with no defects, these magnetic lines will move under the influence of a force exerted on them by the transport current. This motion will dissipate energy, and the heat could make the superconductor go normal. For that reason, it is desirable for a material to contain an optimal array of defects that pin flux lines and keep them from moving. Energetically, it is more stable for a magnetic flux line to sit on a defect than away from the defect; that's pinning. To maximize a superconductor's current-carrying capacity, we should optimize the defect structure to ensure good flux pinning. At present, we are just trying to determine which defects are important for maximizing pinning and current-carrying capacity. Recently, as part of our collaboration with IBM, we discovered that line defects, called linear defect tracks, which are produced by heavy-ion irradiation damage, can dramatically increase the J_c of single crystals. The flux pinning by the tracks is extremely strong and orientation dependent because both the tracks and flux lines are linear structures. The Holifield Heavy Ion Research Facility at ORNL was used for this work, which is an example of the multidisciplinary approach of the Pilot Center. ornl

For more information, call David Christen at 615-574-6269.

HURDLING THE BARRIERS

The Supercon



ducting Motor

Admiring an early model of the new superconducting motor are several of its developers (from left)—Bob Hawsey of ORNL's Applied Technology Division, Ben McConnell of the Energy Division, Milton Bailey of the University of Tennessee, and Bill Schwenterly of ORNL's Fusion Energy Division.

A superconducting motor based on a new design has been built and operated by ORNL researchers. The only operating large alternating-current superconducting motor in the United States, the device shows that new materials and power electronic controls can improve the efficiency and vary the speed of the electric motor, a technology that has not changed much in the last 150 years.

The typical electric motor is made of iron components wound with copper wire. The prototype superconducting motor has rotating components fabricated from fiberglass composites, magnets wound with conventional superconducting wires made of an alloy of niobium and titanium (NbTi) and chilled by liquid helium, and a stainless steel and aluminum structure to hold the magnets in place. A long-range goal is to produce magnets with high-temperature superconducting materials and replace the helium refrigerant with a less expensive one, such as liquid nitrogen. Superconductors are materials that lose all resistance to direct electric current flow if chilled to a critical temperature.

One of the findings of the ORNL project is that removing iron from a motor eliminates almost half of the motor's energy losses that result from magnetizing and demagnetizing the iron.

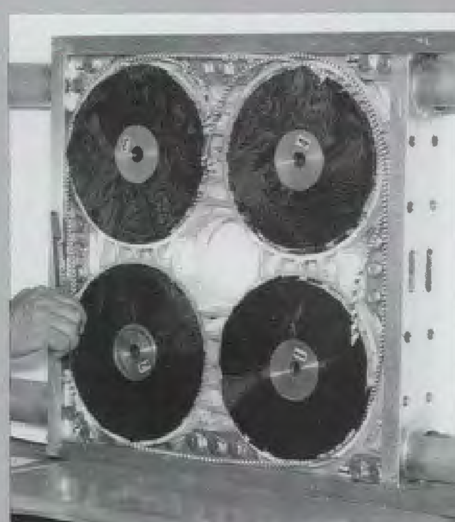
The new motor design was jointly supported by the Department of Energy and the Electric Power Research Institute. About $540,000 in operating and research money was also provided for the project by the ORNL Director's Exploratory Research Fund.

The motor, which is designed to be easily modified for testing, first operated on September 21, 1990. This research event was witnessed by some of the key researchers responsible for the prototype development: Bob Hawsey, Applied Technology Division; Ben McConnell, Energy Division; Keith Kahl, Engineering Technology Division; Bill Schwenterly, Fusion Energy Division; Carl Sohns, Instrumentation and Controls Division; and J. Milton Bailey of the University of Tennessee.

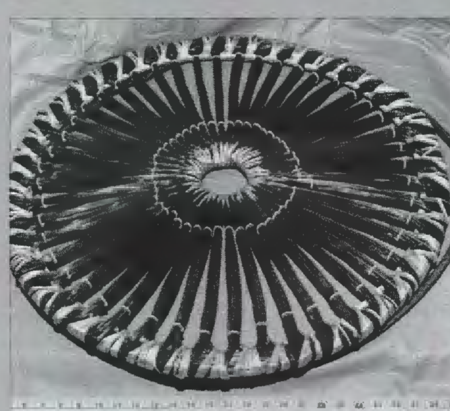
A few weeks later, a superconducting motor demonstration was held for the local press. Reporters were told that 64% of the electricity generated in the United States is consumed by electric motors 20 hp or larger and that an efficiency increase of as little as 3 to 4% in all motors larger than 20 hp could save billions of dollars per year. The annual U.S. electrical energy consumption would be reduced 2% if large-motor efficiency increased 3%.

A superconducting motor would be more energy efficient than a conventional electric motor for at least two reasons. Because the superconducting wires in the stationary magnets offer no resistance to direct current, the motor would consume less electricity. In addition, because the magnetic field of the superconducting magnet can be made stronger than that of a conventional copper-wire–wound

"A superconducting motor would be more energy efficient than a conventional electric motor."



These four superconducting magnets in a stationary cryostat are a key component of the new superconducting motor.



The armature in the superconducting motor is wound radially with copper wire.

magnet of the same size, the design could be more compact, making the motor smaller and lighter. Large amounts of electricity and money would be saved if superconducting motors were used in huge machines, such as aluminum or steel rolling mills, large pumps, and fan motors.

An electric motor is a machine for converting electrical energy into mechanical energy. Conventional motors are based on an invention in the 1840s by American physicist Joseph Henry, who showed that electric current could be used to spin a wheel for operating a machine.

When an electric current is passed through a component wound with wire located within a magnetic field, the current in the conducting wire interacts with the existing magnetic field, causing the component to move.

The superconducting motor developed at ORNL consists of a drive shaft holding a rotating armature, which is powered by alternating current (setting up a rotating magnetic field), and a stationary cryostat containing four superconducting field coils, which are energized by direct current. Each of two rotating armature assemblies sandwiching the cryostat are wound with radially conducting copper wires (like spokes on a wheel). The interaction of these currents and the magnetic fields, which are parallel to the axis of rotation, cause the armature assemblies to turn the drive shaft. Because the magnetic field from the superconducting field coils is parallel to the axis of rotation, the new device is described as an axial-air-gap motor. It is theoretically capable of producing 100 hp at 1800 rpm. However, the motor uses an adjustable-speed drive and produces a

Bob Hawsey inspects components of the axial gap superconducting motor.

controlled speed and horsepower. Previous superconducting motor designs have been limited to the direct-current homopolar and alternating-current synchronous motor designs.

The design of the new motor keeps the axial air gap—the distance between the armature and the field coils—as small as possible to improve operating efficiency in a magnetic field of 2.2 tesla. The designers made the axial gap smaller (2 in.) than that of earlier superconducting motor designs by placing the structure that keeps the field coils from moving as a result of magnetic field stresses outside the air gap. In addition, the designers replaced the iron with plastic composites in the armature. However, because no iron is present, the magnetic field is not uniform, thus reducing the motor output somewhat.

Plans call for placing iron in the static direct-current field. This addition would not increase the motor's losses significantly, but it would improve its operating power levels. Present motor output is limited by current spikes that cut off the system protecting the power electronics for the adjustable-speed drive. This problem results from the low inductance of the armature. The drive is an older model configured to operate a conventional motor with significantly higher armature inductance. Inductance is a measure of the voltage resulting from a variation of the current in an electrical circuit.

To solve this problem, the researchers plan to initially add inductance external to the motor and to redesign the drive to electrically match the motor's operating characteristics near the cryostat to provide electrical inductance, which stabilizes magnetic fields.

Ultimately, this advanced electric motor will have its own "automatic transmission," thanks to an advanced adjustable-speed drive under development at ORNL. The addition of these power electronics increases the overall system efficiency in applications that require external gearing.

Further development of this device should lead to electric motors that are smaller and lighter and use less energy than the motors of today.—*Carolyn Krause*

Waste Site Remediation: Are We Doing It Right?

By Curtis C. Travis

Some organizations, such as ORNL, are discovering that some local groundwater is contaminated and that it cannot be completely cleaned up. To determine whether an area has contaminated groundwater, monitoring wells must be installed. At ORNL about 200 groundwater-quality monitoring wells have been installed at the perimeters of 11 waste area groupings. The procedures used in installing 170 of these wells are shown in the photographs accompanying this article.

To remove any contaminants present, drilling tools are sandblasted before being used for well drilling at ORNL.

Hundreds of waste sites in the United States have long been considered potentially threatening to public health and the environment. For ten years, a mechanism has been in place by which the U.S. Environmental Protection Agency (EPA) could address the problem of hazardous waste sites as part of its mission to protect the public health and environment. In 1980, Congress passed the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA, or Superfund), authorizing $10 billion for the identification, evaluation, and remediation of the most hazardous sites. In 1986, the Superfund Amendments and Reauthorization Act (SARA) was passed to give the EPA additional resources and direction for remediation of hazardous waste sites. Critics have argued, however, that the EPA has failed to implement an aggressive program that protects human health and the environment and that the decision-making approach for selecting sites for cleanup is ill-defined and lacking in clear priorities.

In ORNL's Center for Risk Management, Carolyn Doty and I have conducted a series of analyses on the effectiveness of cleanup decisions made by the EPA. In our analyses, we have become aware of two misconceptions regarding hazardous waste site remediation. The first misconception is that all Superfund sites selected for cleanup pose a serious risk to public health. The second misconception is that contaminated aquifers can be restored to drinking-water standards. Our conclusions have prompted the National Academy of Sciences to propose a study on the issue of reducing health risks from groundwater contamination.

Decision Process Flawed

CERCLA mandated that the EPA develop a list of the nation's worst hazardous sites based on relative risk. More than 1200 sites have been placed on the National Priorities List (NPL) for cleanup, including 13 sites in Tennessee, one of which is the Oak Ridge Reservation. The estimated cleanup costs for these sites range from $32 billion to $80 billion, excluding Department of Energy sites. We found, however, that the process by which the sites are placed on the NPL and remedial alternatives are selected for the sites is flawed.

EPA developed the Hazard Ranking System (HRS) for placing and ranking sites on the NPL. To determine if the proper sites have been placed on the NPL, we studied the correlation between HRS scores and actual risk levels at hazardous wastes sites where risk levels were later estimated. We found poor correlation between the scores used to place the sites on the NPL and the actual risk levels at the sites.

Our analysis suggests that most of the sites on the NPL pose little or no current risk to public health. The possibility also exists that many sites that do present a health hazard may not be included in the Superfund program. In fact, a report from the Senate Budget Committee states that more than 425,000 toxic waste sites are potential Superfund sites but that the EPA has given priority listing to only about 1200.

In September 1990, Senator James Sasser of Tennessee, who heads the Senate Budget Committee, cited the report's finding that only 4%, or 52, of the nation's 1200 priority sites have been cleaned up in the first 10 years of the Superfund program. He said that many of the most hazardous sites "are being left to fester year after year." The senator called for a new approach before billions of dollars are poured into the program.

The Sasser report supports a general belief that large numbers of people are being exposed to elevated health risks at Superfund sites. The facts do not substantiate this viewpoint. A study completed in 1990 by the Agency for Toxic Substances and Disease Registry found that only 11.5% of the 950 sites on the NPL pose actual or potential current risk to public health.

Once a site is on the NPL, the likelihood that it will be remediated is great. Although approximately 88% of the sites we reviewed were remediated, little correlation existed between risk levels and remediation decisions. Risk assessment is being used to determine baseline risk at most Superfund sites. However, about 75% of the sites fall in a gray area, where, to be conservative, sites are considered to be potential hazards to public health because the data needed to verify that they are not dangerous are unavailable. Thus, most of the decisions to remediate these sites are based on the existence of contamination per se and not on current public health risk.

In addition to setting clear priorities for selecting sites for cleanup, the selection of effective remedies is essential. Many remedial alternatives have been selected despite inadequate evidence that they can effectively and permanently decontaminate sites that pose an urgent threat to human health. We found that one of the ineffective remedial actions selected for many sites is the "pumping and treating" of groundwater with the objective of restoring an aquifer to drinking-water standards.

"We found that one of the ineffective remedial actions selected for many sites is the 'pumping and treating' of groundwater."

Groundwater Cleanup Problems

Environmentalists and EPA managers generally believe that aquifers at Superfund sites can be restored through groundwater "pumping and treating." This expensive and widely used approach involves pumping water from the ground, removing the organic contaminants by air stripping or other treatment methods, and discharging the decontaminated water into surface streams or reinjecting it back into the ground. *(Continued on p. 32.)*

Rick Herron and James Shelton, both of Geotek Engineering, collect a soil sample during auguring as ORNL health physicist Carl Stooksbury (right) checks the sample for radioactive contamination.

Preparing to drill through rock, Steve Clark (left) and Steve Kirk connect an air rotary rig to a containment box designed by Energy Systems engineers. The trailer-mounted tank holds cuttings and water generated during air rotary drilling and filters the exhaust in case contaminants are present.

Bryn Howze (left), hydrogeologist with ERC Environmental and Energy Services Company, and Rick Pickel, driller with A. L. Clark Drilling Company, add bentonite pellets to the annulus of a shallow well under construction. The pellets form a seal between layers of sand and grout, which prevents surface water from entering the well.

The completed well has a steel protective casing, a padlocked cap, a concrete pad, and steel guardposts. Information about the well's construction and subsequent sampling can be tracked using the well number on the name plate.

"We believe pumping and treating should be used only to keep the contaminated groundwater from spreading."

Our review of recent theoretical studies and field experience shows that pumping and treating for aquifer restoration to drinking-water standards, an objective at 68% of Superfund sites, is infeasible. Thus, we believe pumping and treating should be used only to keep the contaminated groundwater from spreading.

Recent groundwater transport modeling indicates that groundwater pumping is essentially ineffective. Leading groundwater scientists have predicted that continuous pumping for as long as 100 to 200 years may be necessary to reduce contamination to 1% of current levels at many sites, assuming the ideal conditions in which contamination is totally dissolved in a homogeneous aquifer.

Aquifer restoration is less reliable at sites involving non-aqueous phase liquids (NAPLs) that either float on top of the water table or sink to the bottom of the aquifer. A past director of EPA's groundwater research laboratory in Ada, Oklahoma, has noted that restoration could take thousands of years for water-insoluble constituents such as jet fuel. When large pools of dense NAPLs are present at the bottom of an aquifer, meeting drinking-water standards is unachievable at any cost. At best, even if eventual restoration is conceivable, it is impossible to predict how long pumping and treating will take to restore an aquifer. In spite of this observation, aquifer restoration is the remedial objective at approximately 93% of the sites that are known to involve NAPLs.

Further proof of the ineffectiveness of pumping and treating for aquifer restoration comes from direct experience in pumping contaminated aquifers over the past ten years. A recent EPA study involving 19 sites where pumping and treating had been under way for up to ten years concluded that, although significant amounts of contaminants had been removed, little success had been achieved in reducing contaminant concentrations to the target levels. Typically, the concentrations initially drop by a factor of 2 to 10, followed by a leveling out with no further decline. The problem is exacerbated once the pumps are turned off because contaminant levels begin to rise again.

An interesting example is the IBM Dayton hazardous waste site in New Jersey. Groundwater at the site was contaminated with ~400 gal of volatile organic compounds (VOCs), primarily 1,1,1-trichloroethane (TCA) and tetrachloroethylene (TCE). The maximum groundwater concentrations ranged from 9590 parts per billion (ppb) for TCA to 6132 ppb for TCE. Pumping with an average on-site extraction rate of 300 gal/min between 1978 and 1984 lowered VOC concentrations to below 100 ppb. However, in 1988, four years after shutdown of the operation, TCE concentrations rose to 12,558 ppb. Pumping was resumed in 1989, but the remedial objective was changed from restoration to containment. Thus, despite extensive groundwater pumping, this site is no closer to remediation than it was 12 years ago.

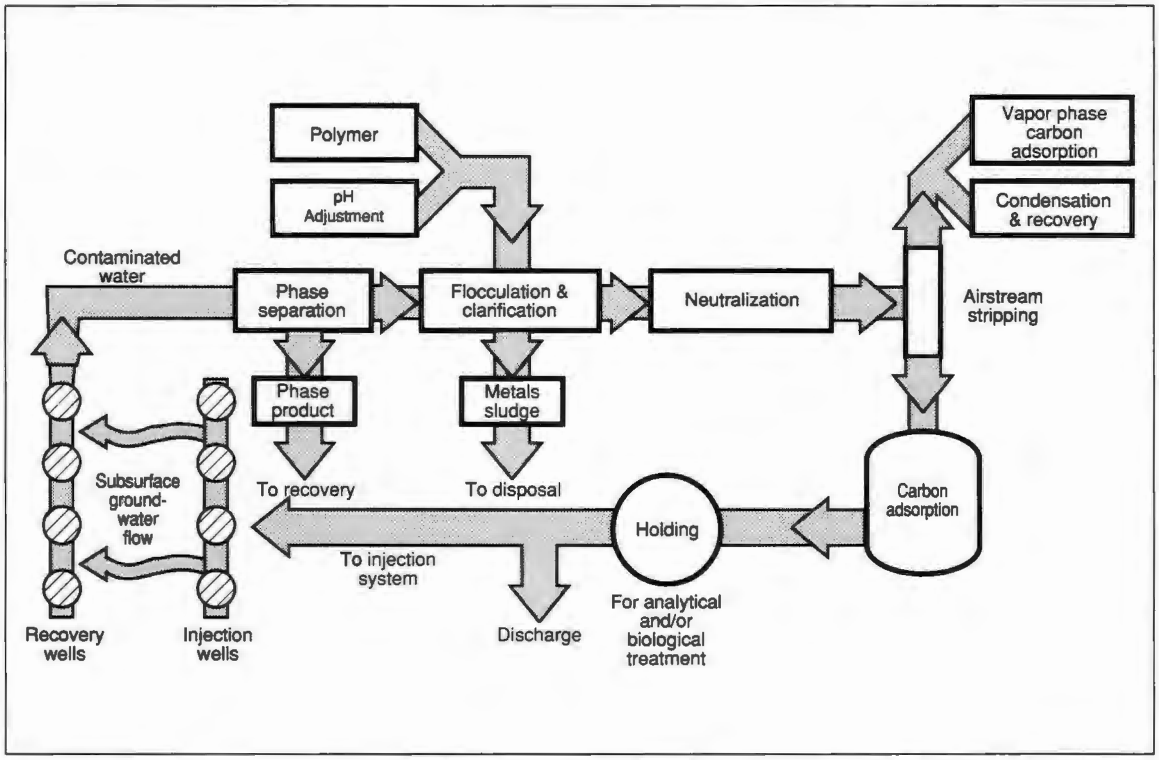
It is reasonable to conclude from scientific evaluations of the effectiveness of pumping and treating groundwater for aquifer restoration that drinking-water standards cannot be met and that containment is, in most cases, the only feasible alternative. Despite this evidence, the majority of cleanup strategies for hazardous waste sites include the pump-and-treat remedy for groundwater restoration.

Recommendations

The Superfund program has failed to set realistic, well-defined goals. Clear priorities have been lacking in the selection of sites to remediate and decisions about the degree of remediation required. Many remedial actions selected do not offer an effective and permanent solution; therefore, money is being spent on actions that do not guarantee protection of public health and the environment.

Decision making concerning site cleanup has been ambiguous regarding risk. Many sites being cleaned up have not been shown to pose public health or ecological risks. The decisions to clean up sites and the remedies selected appear to be influenced more by the presence of contamination per se, the cost of remediation, compliance with state and federal environmental regulations, and professional judgment than by information about health risks.

To meet the challenge of effectively remediating hazardous waste sites, we recommend an enhanced



Schematic of a pump-and-treat system for removing contaminants from groundwater.
Source: O. H. Materials Corporation

commitment to addressing the "worst sites first" and to developing and selecting effective and permanent remedial actions. Emphasis should be placed on (1) immediately identifying and remediating sites that pose a clear and present risk to human health, (2) establishing realistic cleanup goals given the current state of technology, and (3) matching the extensiveness of remediation with the degree of current and future risk. For example, it should be acknowledged that aquifer restoration is not currently technically feasible and that restoration of the environment to a pristine state is not always necessary to ensure protection of public health and the environment.

We also recommend accelerated research aimed at demonstrating the effectiveness of different treatments under various field conditions. Environmental variables (e.g., soil type, pH, microbial content) should be considered in predicting the relative effectiveness of various remedial actions. Such information could guide in selecting the most effective of possible remedial actions.

The focus should be on remedies that will reduce or eliminate contamination permanently. Groundwater pumping and treating can be used to contain contaminated groundwater, but this approach is ineffective for completely removing contamination from groundwater. Because restoring groundwater to a condition that meets health-based standards is difficult using the conventional approach, remedial efforts should focus on developing and implementing permanent cost-effective source control remedies.

In short, the highest priority in dealing with our nation's hazardous waste sites should be to identify sites that pose a clear and immediate threat to human health and the environment and then to remediate them with proven and effective technologies.

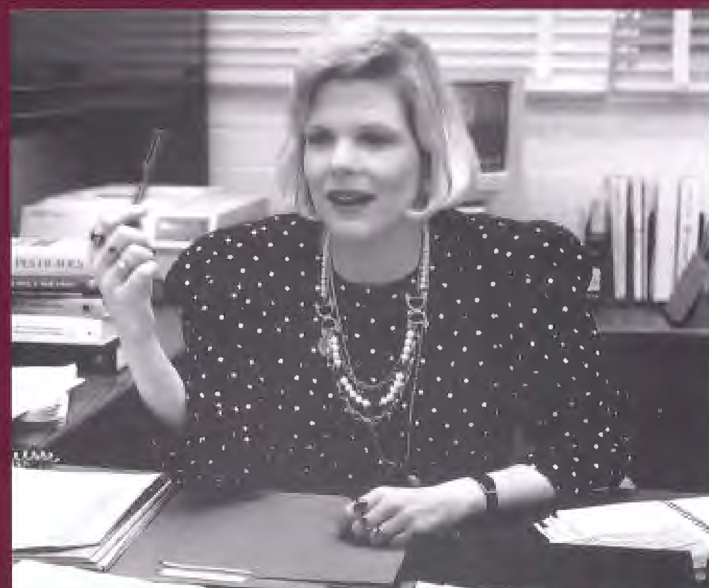
For more information, contact Curtis Travis at 615-576-2107.

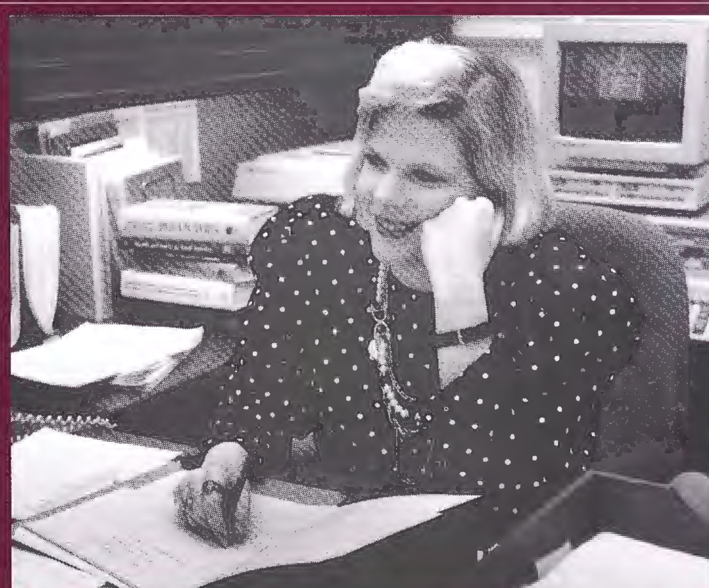
Biographical Sketch

Curtis C. Travis is director of ORNL's Center for Risk Management, president of the National Society for Risk Analysis, and editor-in-chief of *Risk Analysis: An International Journal.* In 1971 he received his Ph.D. degree in applied mathematics from the University of California at Davis. He worked as a research engineer at the Jet Propulsion Laboratory of the California Institute of Technology from 1966 through 1968 and taught engineering and applied mathematics at Vanderbilt University (1971–1974) and the University of Tennessee (1974–76). He joined the ORNL staff in 1976.

Travis is also chairman of the Office of Science and Technology Policy Task Force on Risk Analysis in Federal Agencies, a member of the Science Advisory Board for the National Center for Toxicological Research, and a member of the Scientific Advisory Panel on the Federal Insecticide, Fungicide, and Rodenticide Act for the U. S. Environmental Protection Agency. He collaborated with the Agency for Toxic Substances and Disease Registry in production of their Guidance Document for Health Assessments at Superfund Sites. Here, he and his colleague Carolyn Doty review a report on waste site remediation.

"No Option Would Satisfy Everyone"





Last year Robin White, environmental risk coordinator for the Environmental Restoration Division of Martin Marietta Energy Systems, Inc., faced a tough challenge. She tried to convince attendees at a meeting that there is no easy answer to the problem of groundwater cleanup.

"The public has one perception about the environmental problem of hazardous waste; the scientists have another."

"They wanted to know about environmental problems and I viewed it as an experiment in education," she said. "The public has one perception about the environmental problem of hazardous waste; the scientists have another perception; and the regulators have an even different perception, which is an amalgamation of the other two perceptions. None of them have come to grips with the fact that every group has its own agenda and that our choices for dealing with these problems are limited and have trade-offs."

Addressing some 80 registered sanitarians and restaurant inspectors at a National Environmental Health Association meeting in Charlotte, North Carolina, she talked about alternatives for dealing with groundwater contamination. She presented the audience with an example from a group of actual sites that the Center for Risk Management has studied. The site was described as a large industrial facility whose past practices had contaminated groundwater. She told them that the groundwater plume was currently confined within the facility boundaries and was not used as a source of drinking water for workers or the public. She explained that contaminants fell into two categories: highly soluble, noncarcinogenic materials, which were the major contaminants, and less soluble, carcinogenic agents, which were present in much lower levels.

"First I explained that one option was to leave the contaminated groundwater there. I discussed with them results of model simulations that indicate that the highly soluble contaminants would be 'washed out' of the watershed in 20 to 30 years. The less soluble, cancer-causing agents were predicted to adsorb to the soil and stay there.

"I also reminded them that an advantage of the no-action alternative is that it costs nothing, unless there is the possibility of regulatory fines, for example."

White said most members of her audience were not pleased with this no-action option because they felt it did not address the problem. So she offered an alternative.

"What if we put a cap on it to keep rainwater from percolating into the system? The cap prevents the groundwater plume from getting larger and spreading. The cap is relatively inexpensive to install and maintain—about $3.5 million—and has few environmental side effects."

Most members of the audience liked this option better than doing nothing, despite the cost. But White learned they were still not convinced that this was the best choice, because the cap did not appear to be a very aggressive course of action. So she presented another, more aggressive option: remove the source by excavating the contaminated soil and materials from the original source area.

"What if we remove contaminated materials and soil and move them to an engineered concrete facility. Is it acceptable if we construct the facility in your county? And are you willing to pay extra taxes to build and operate such a facility?" Although most members of the audience liked the more aggressive approach that excavation offered, the combination of cost and the Not In My Back Yard Syndrome made this alternative also unpalatable to them.

Finally White told them, "We could construct and operate a facility to 'pump and treat' the groundwater—extract it from the ground, remove contaminants from the water, and discharge the water to surface water or reinject it into the ground. Our best information and simulations indicate that this approach would remove most of the contaminants. However, it could also dewater the local watershed for several kilometers, possibly resulting in dangerous subsidence and the loss of habitat for certain species. The treatment modules would produce from 5000 to 25,000 lb of calcium carbonate sludge per day, which would have to be disposed of as mixed waste because some radioactivity would be present in the sludge. The cost of a pump-and-treat strategy could range from $20 million to $100 million, depending on how aggressive an approach is implemented."

White then pointed out that costs for such an alternative would ultimately be borne by taxpayers—all in an era when many communities cannot afford to pay the taxes required to support basic services such as police and fire protection and education.

Despite the environmental risks and exorbitant costs, the audience initially found this proposed action appealing because it showed a willingness to grapple with a difficult problem. However, their enthusiasm for this approach dwindled after White gave the results of a risk assessment of all the alternatives.

"We found that after 20 years of doing nothing at the site, the quality of the groundwater would be below drinking-water standards. After 20 years of using the cap, groundwater quality would still be below drinking-water standards. And after using the pump-and-treat strategy for 20 to 30 years, the quality of the underground water would also be below drinking-water standards. Further, none of the alternative actions reduced the cancer risks at the site significantly lower than that achieved through the no-action alternative."

She told the audience that those were the main choices and that new approaches, such as in situ vitrification and genetically engineered organisms that feast on contaminants, were being studied but have not yet been shown to work or to be environmentally acceptable.

White said her audience was suddenly confused and frustrated by the lack of good choices. "Now you know what makes my job a dilemma," she said. "We can do the risk analysis and evaluate our options. But we can't choose an option for addressing problems at hazardous waste sites that will satisfy everyone."—*Carolyn Krause*

Enzymes for Extracting Energy from Trash

By Jonathan Woodward

"If today's American newspaper waste were 'enzymatically hydrolyzed' to glucose and then fermented to ethanol, over two billion gallons of fuel could be generated each year."

Knox County's only landfill will be full by the early 1990s. In the future, much of the sort of waste shown here may be recycled or converted to fuel, thus extending the lives of landfills.

The garbage we generate every day contains considerable potential energy, but instead of using it, we dump it into landfills. This garbage biodegrades very little, even after 20 years. As the price of energy has risen, however, scientists have been searching for ways to extract energy from trash. At least 40 to 50% of domestic garbage contains cellulose, a complex carbohydrate that could be converted to liquid fuel. Examples of such energy-rich, cellulosic trash are newspapers, cardboard, disposable diapers, vegetables, junk mail, old clothes, and tree leaves.

Producing inexpensive energy from trash rather than burying it would have a double benefit. The liquid fuel produced could be used in automotive vehicles, replacing gasoline made from imported oil. Furthermore, reducing the amount of garbage delivered to landfills could delay the closure of many of the nearly full ones and slow the rising costs of landfill disposal.

Every year in the United States, 30 million tons of newspaper are produced. Most newspaper ends up in landfills, occupying 10 to 28% of the landfill volume. An attractive alternative to burying the newspapers, besides recycling, is to produce energy from this cellulosic waste. The energy content of cellulosic waste (4×10^{-9} quads per ton, 1 quad = 10^{15} Btu) can be released by burning it, but cellulose incineration is environmentally unacceptable because it releases toxins into the environment. No device has been developed to control toxic emissions from cellulose incinerators adequately and economically.

Another way to produce energy from cellulosic waste is to employ special enzymes to break it down into its principal component—a simple sugar called glucose. The glucose could then be fed to microorganisms that can convert it into chemicals and alcohol fuels. For example, if currently generated today's American newspaper waste were "enzymatically hydrolyzed" to glucose and subsequently fermented to ethanol using yeast, over 2 billion gallons (70 million cubic meters) of fuel could be generated each year.

Professor Herbert Klei of the University of Connecticut, Storrs, supports the use of ethanol as an alternative to gasoline. The service station is near Maringa, Brazil.

In addition to domestic cellulosic wastes, other ubiquitous sources of cellulose in the world that could replace fossil fuels as our primary source of energy include woody biomass (trees) and agricultural wastes (wheat straw, corncobs, and rice and oat hulls). Seasonal sources of cellulose are tree leaves and grass cuttings.

With my colleagues in the Chemical Technology Division, I have been studying the mixture of enzymes called cellulase since joining ORNL in 1980. Cellulase enzymes, which are types of protein, can break down cellulose into sugars for fermentation into alcohol fuels. The ultimate goal of our research is to reduce the dependency of the United States on foreign sources of energy, which are very uncertain, through the understanding of cellulase enzymes and their application to energy production.

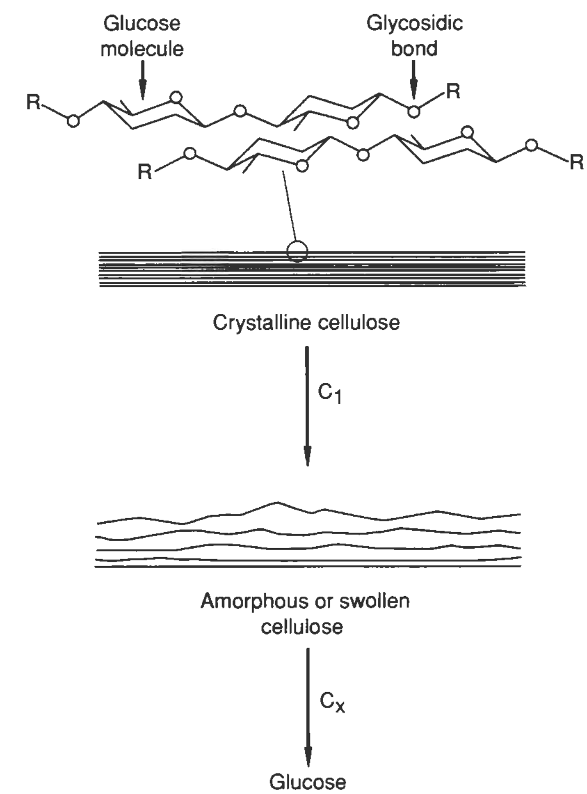
Discovery of Cellulase

During World War II, the U.S. Army was concerned about the rotting of military clothing and equipment in the jungles of the South Pacific and sought the cause. Research conducted by the Army at the Natick Development Center in Massachusetts led to the isolation of the culprit; a rotted cartridge belt found in New Guinea yielded a fungus that was identified as *Trichoderma viride*. The primary constituent of the cartridge belt—cellulose—provided the energy source for the growth of the fungus. An enzyme complex called cellulase, which was secreted by the *T. viride* growing on these moist cellulosic materials, chemically stimulated the breakdown of cellulose into glucose. The fungus absorbed the glucose and converted it into chemical energy through a series of biochemical reactions.

During the 1950s, '60s, and '70s, Elwyn Reese and Mary Mandels at the Natick laboratories contributed greatly to our knowledge about the mechanism by which the enzyme cellulase catalyzed the hydrolysis of cellulose to glucose. In the late 1970s *T. viride* was renamed *T. reesei* in honor of Reese.

Reese's Hypothesis

Simply stated, cellulose is a complex carbohydrate—a compound made of carbon, hydrogen, and oxygen $(C_6H_{10}O_5)_x$. Technically



In Reese's C_1-C_x hypothesis explaining the action of cellulase on crystalline cellulose, C_1 acts on tight bundles of cellulosic chains held together by hydrogen bonding, rendering them susceptible to the action of cellulase (C_x). Although the identity of C_1 is still unknown, it is believed to be a function of the CBH (and possibly EG) component of cellulase resulting from its adsorption to the cellulosic surface.

speaking, it is a polysaccharide, which is a large, complex molecule that can be decomposed by hydrolysis into its constituent glucose molecules. Hydrolysis is the chemical process of decomposition in which chemical bonds are broken and the elements of water are added to the final reaction product. Cellulase is a catalyst in this reaction because it stimulates the process of breaking down the large molecules of cellulose (also called sugar polymers) into smaller glucose molecules.

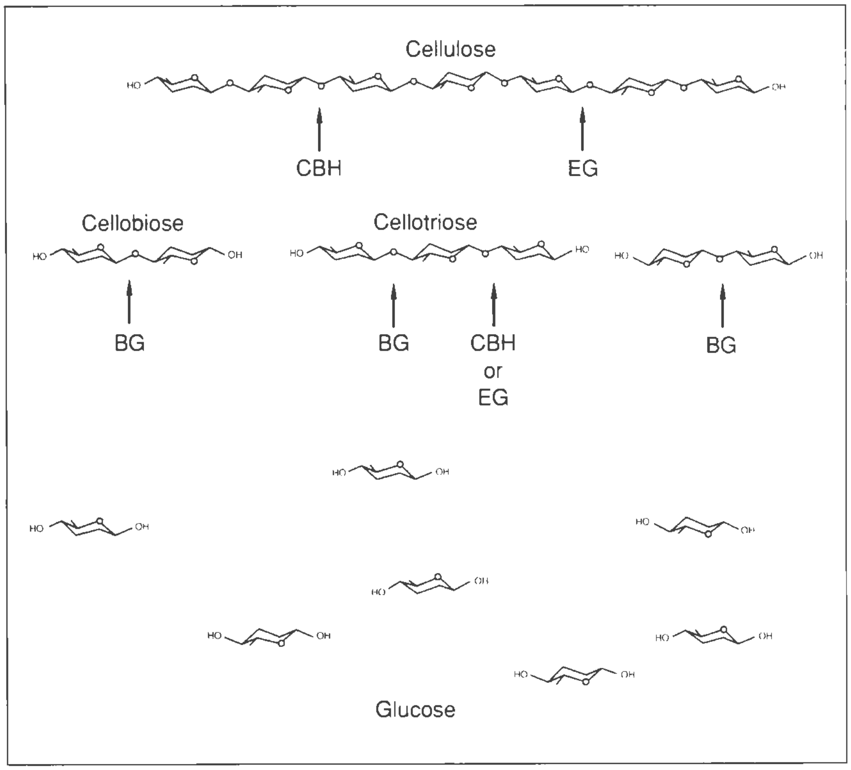
In its native state, crystalline cellulose is composed of parallel or antiparallel fibril chains that are held together in tight bundles by hydrogen bonds. Cellulose is completely insoluble in aqueous media, but acid treatment or a chemical modification render it noncrystalline, or amorphous. In 1950 Reese observed that two groups of cellulase-producing fungi exist, but they differ in their hydrolysis abilities. Both groups were found to produce the cellulase enzyme that can hydrolyze glycosidic bonds (the covalent bonds linking pairs of glucose residues) in amorphous cellulose [e.g., carboxymethyl-cellulose (CMC)]. However, Reese observed that only a limited number of fungi (e.g., *T. reesei, T. koningi, Fusarium solani, Penicillium funiculosum, Sporotrichum pulverulentum*, and *Talaromyces emersonii*) produce cellulase enzymes that can hydrolyze naturally occurring crystalline celluloses, such as cotton. This discovery prompted Reese to propose his C_1-C_x hypothesis to explain the difference.

Basically, the hypothesis states that cellulases capable of hydrolyzing naturally occurring cellulose require a factor (C_1) that renders cellulose susceptible to the hydrolytic action of C_x that results in glucose formation. The role of C_1 would be to separate individual cellulose chains from bundles of crystalline cellulosic fibers so that they could be hydrolyzed by C_x. Reese proposed that those cellulases unable to hydrolyze naturally occurring cellulose lack C_1. His hypothesis was the primary impetus for the next four decades of research, dedicated to understanding the mechanism by which cellulases catalyze the hydrolysis of naturally occurring cellulosic materials to glucose.

Cellulase Composition, Structure, and Function

Cellulases produced by "cellulolytic" fungi are composed of three main types of enzyme components: cellobiohydrolase (CBH), endoglucanase (EG), and ß–glucosidase (BG), based upon their catalytic activity. Both CBH and EG adsorb to the cellulose surface, and their action results in the formation of cellobiose (paired glucose molecules called dimers) and single glucose molecules. BG catalyzes the hydrolysis of cellobiose to glucose; it does not need to adsorb to the surface of cellulose because cellobiose is a soluble sugar. The names of CBH and EG are based on their mechanistic action. The main product resulting from the action of CBH on different celluloses (e.g., cotton, cellulose powder, acid-swollen cellulose) is cellobiose, which is released from the chain ends of cellulose. EG acts upon the amorphous cellulosic materials—CMC and acid-swollen cellulose—in random fashion, catalyzing the hydrolysis of internal glycosidic bonds, resulting in a rapid decrease in chain length and the generation of soluble sugars (e.g., tetramers, trimers, and dimers of glucose, and glucose itself). The BG component completes the hydrolysis of these soluble sugars, primarily cellobiose, to glucose.

With regard to Reese's hypothesis, the EG component is accepted to be C_x and CBH to be C_1 because the cellulases of fungi that act only upon noncrystalline CMC and acid-swollen cellulose lack CBH. The release of individual chains from crystalline cellulose bundles has not been observed to date, but recent advances in characterizing the structure of the CBH and EG components may shed some light on this phenomenon.



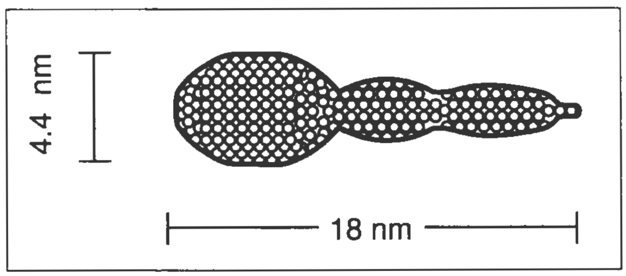
In this schematic of how cellulase components work, CBH and EG adsorb to the cellulosic surface, where CBH removes cellobiose units. EG acts internally, depolymerizing the chain and generating new ends for the action of CBH. BG hydrolyzes cellobiose to glucose.

CBH's Tadpole Shape

Research by Marc Claeyssens in Grent, Belgium, and Göran Petterson in Uppsala, Sweden, has led to the discovery that both the CBH and EG components of cellulase possess a common structural organization and consist of two distinct domains—a catalytically active "core" and a cellulose-binding domain. Most of our present knowledge about the detailed structure of these enzymes comes from studies of the CBH component, which makes up about two-thirds of the total protein in cellulase. Small-angle X-ray scattering studies by Hermann Esterbauer in Graz, Austria, have revealed that the major *T. reesei* CBH component is shaped like a tadpole; the head forming the catalytic "core" is made up of approximately 420 amino acids (the basic building block of proteins), and the tail, or cellulose-binding site, consists of 36 amino acids. The two domains are linked by a short sequence of amino acids. If the tail of CBH is cut off using a proteolytic enzyme called papain, its ability to adsorb to and, hence, hydrolyze insoluble cellulose is drastically reduced, but it retains all its catalytic activity toward small synthetic soluble cellulose substrates.

Per Kraulis at the National Institutes of Health, in collaboration with others, published the structure of the CBH tail that was determined using two-dimensional nuclear magnetic resonance and showed it resembles a compact wedge whose shape is maintained by hydrogen bonds and two disulfide cross-links that occur between four residues of the amino acid cysteine. However, it has yet to be shown whether the binding of this wedge-shaped tail to the cellulose surface results in the prying apart of individual chains from the bundle of cellulosic fibers. Because the CBH and EG components have a common structural organization, it will also be interesting to determine whether the wedge-shaped tail is common to both. C_1, therefore, may not be CBH per se but rather a property of CBH and EG—namely, the ability to adsorb on cellulose and, perhaps, by some unknown mechanism, to pry open the cellulosic fibers and release the chains for hydrolytic action.

"Small-angle X-ray scattering has revealed that the major T. reesei *CBH component is shaped like a tadpole."*



The tadpole shape of CBH as suggested from small-angle X-ray scattering studies. Reprinted with permission from Schmuck et al., *Biotechnol. Lett.* **8**, 379. Copyright 1986, *Science and Technology Letters.*

During the summer of 1990, a group led by Alwyn Jones in Uppsala, Sweden, published a paper on the three-dimensional structure of the catalytic "core" of a CBH molecule from *T. reesei*. The active site of this enzyme (i.e., the part directly involved in the catalytic mechanism) was shown to be located in an enclosed tunnel-like structure. The fascinating aspect of this finding is that it now becomes easy to imagine and explain how cellobiose units of individual cellulose chains entering the tunnel are sequentially removed from the chain ends.

Research Progress at ORNL

For the past 11 years, I have been studying cellulase at ORNL with the aim of overcoming one of the problems that would be associated with the industrial-scale use of cellulase for cellulose hydrolysis. That problem is finding a way to produce the large amount of cellulase enzymes needed to achieve large-scale conversion of cellulose to glucose. In fact, enzyme production accounts for as much as 60% of the total processing costs of turning cellulose into glucose. Several approaches have been taken to solve this problem, including (1) recovering and reusing the enzyme after the hydrolysis is completed, (2) using the enzyme more efficiently to reduce the amount needed, and (3) generating cellulase components having enhanced specific activity, again to reduce the amount of enzyme required.

Most enzymes can be recovered and reused because they can be used in an immobilized form (i.e., chemically or physically attached to, or entrapped within, a water-insoluble support). The use of the CBH and EG components in an immobilized form, however, is not regarded as practical because effective interaction between immobilized CBH-EG and insoluble cellulose cannot occur. Reversibly immobilized CBH-EG, where the enzyme components desorb from the support in the presence of cellulose and readsorb back at the completion of hydrolysis, may be practical, especially if pure cellulose is hydrolyzed.

At ORNL we have developed a U.S.-patented method for recovering cellulase from a reaction mixture based upon the use of adsorbent granules. Unlike the CBH-EG components, BG can be used in immobilized form because the substrates upon which it acts are soluble and, therefore, can diffuse into the microenvironment of the support to interact effectively with the enzyme. We have successfully immobilized BG by covalent bonding and adsorption to water-insoluble, carbohydrate-derived polymers and have shown that the immobilized preparations are able to hydrolyze cellobiose efficiently. They can also be made to possess higher operational stability than the naturally occurring enzyme if BG is subjected to a simple chemical modification procedure (involving intramolecular cross-linking) before immobilization. Such immobilized and stabilized BG preparations have also been entrapped in propylene alginate–bone gelatine gel spheres (2–3 mm diam). In this form they can be used in a variety of different reactor configurations for the continuous hydrolysis of cellobiose to glucose. As far as we know, BG is the first enzyme component to be entrapped in these particular spheres, which have a special advantage over other kinds of gel spheres (e.g., calcium alginate): they do not require the external introduction of ions to maintain their structural stability.

Michele Clarke, a teacher research associate from Marquette University High School, Milwaukee, prepares gel-entrapped ß-glucosidase that can be used repeatedly for cellobiose hydrolysis.

"The problem is finding a way to produce the large amount of cellulase enzymes needed for large-scale conversion of cellulose to glucose."

If cellulose is not completely hydrolyzed to glucose in an industrial process or if "real" cellulosic residues are being hydrolyzed (as in newspaper, which can contain up to 30% lignin–aromatic polymers complexed with cellulose), then the CBH-EG components will mostly remain adsorbed to the residual cellulose or lignin. To be recovered and reused, they must be desorbed from the residues. Protein denaturants such as urea and guanidine hydrochloride can be used to desorb cellulase components from cellulosic residues. Although the catalytic activity of the cellulase components is lost by this treatment, we have shown, at least for CBH, that once the denaturant is removed from the enzyme, its ability to hydrolyze cellulose is restored completely. The use of an immobilized BG will prevent the adsorption of this component to lignin.

Another possible way to reduce the enzyme requirement for industrial-scale glucose production is to exploit the phenomenon of synergism that exists between the cellulase components. Individually, the components possess little or no ability to hydrolyze cellulose, depending on the substrate, but in combination with each other, they can effectively hydrolyze cellulose to glucose. This synergy, as we found, is greatest when

Jodi Tate, an Oak Ridge Science and Engineering Research Semester student from North Dakota State University, purifies CBH using a fast liquid-protein chromatograph.

advances in genetic engineering. The genes encoding both *T. reesei* CBH and EG have been sequenced and expressed in yeast by Jonathan Knowle's group in Espoo, Finland, and Sharon Shoemaker's group in San Francisco. These recombinant enzymes have been shown to possess the ability to hydrolyze different cellulosic substrates.

One approach we are taking at ORNL to reduce the amount of enzyme required is to understand more about the function of the cellulase components in relation to their structure so that methods can be devised to enhance their catalytic activity. Anatole Klyosov of the Soviet Union's Academy of Sciences has shown that the high affinity of an EG component for cellulose in a cellulase complex is correlated with the extensive hydrolysis of crystalline

cellulose is not saturated with the CBH-EG components, but rather when an optimum concentration of each is present. From a practical point of view, approximately 75% of the glucose formed by concentrations of cellulase components sufficient to saturate cellulose can be obtained if they are used at approximately 10% saturation levels. Therefore, if the phenomenon of synergism is used, 90% of the CBH-EG components could be saved for further use, and the resulting glucose concentration would be reduced by only 25%. This reduction could be overcome by increasing the time of hydrolysis.

At first, it may seem rather improbable that purified cellulase components could be used for industrial enzymatic hydrolysis of cellulose. However, such a use is probable because of

cellulose by that complex. If the affinity of CBH and EG components for cellulose can be increased, then greater catalytic activity may result. Thus, less enzyme would be required for a given amount of cellulose hydrolysis.

Currently, no methods have been developed to increase the affinity of a cellulase component for cellulose, but it is possible that chemical modification (using specific reagents or site-directed mutagenesis) of one or more of the amino acids making up the enzyme could achieve this result. The cellulose-binding, or tail, region of a *T. reesei* CBH component is composed of mostly uncharged polar and hydrophobic amino acid groups that interact with the cellulosic surface. Ninety-seven percent of the charged polar amino acids reside in the "core," or head, region. We hope to find out if neutralizing some of these charges in the core would increase CBH's affinity for cellulose. If so, we plan to determine whether the core alone possesses the ability to hydrolyze crystalline cellulose. Such studies could allow us to determine whether the tail of the CBH component merely serves to anchor the enzyme to the cellulose surface or has a specific role in releasing individual chains from cellulose fibers. This, perhaps, would finally lead to the identification of Reese's C_1 factor.

The key goal of cellulase research in the Chemical Technology Division is a better understanding of the mechanism by which the CBH and EG components act together synergistically to hydrolyze cellulosic substrates. These findings could lead to an efficient industrial process for the bioconversion of a variety of cellulosic wastes into valuable chemicals and fuels. ornl

For more information, contact Jonathan Woodward at 615-574-6826.

Biographical Sketch

Jonathan Woodward is a biochemist who has conducted research in ORNL's Chemical Technology Division since 1980. He received his Ph.D. degree in biochemistry from the University of Surrey, United Kingdom, in 1977, and he was a postdoctoral fellow at Vanderbilt University from 1977 to 1980. Author of 50 technical publications and editor of one book, he serves on the Executive Committee of the Division of Biochemical Technology, American Chemical Society, and is also a member of the Biochemical Society of Great Britain. His research interests are enzyme biochemistry and biotechnology for use in energy production and conservation.

RE: Awards & Appointments

Owen Hoffman

Lee Shugart

François Pin

Oak Ridge National Laboratory has received the Aerospace Power Systems Award from the American Institute of Aeronautics and Astronautics for its work in developing fuel cladding and insulation for power systems aboard the *Galileo* and *Ulysses* spacecrafts.

Gordon Fee, former director of ORNL's Engineering Technology Division and former Oak Ridge Y-12 Plant manager, has been appointed senior vice president of Martin Marietta Energy Systems, Inc., replacing **Herman Postma,** former ORNL director who retired January 31, 1991.

A. C. (Tony) Schaffhauser, director of the ORNL High Temperature Superconductivity Pilot Center, is now also associate director of the Conservation and Renewable Energy Program.

C. H. (Winston) Chen has received the Excellence in Research Award of ORNL's Health and Safety Research Division. He was cited for "development of innovative measurement devices including but not limited to new fluorocarbon detectors."

Michelle Buchanan has been elected treasurer of the American Society for Mass Spectrometry, member of the Advisory Board of the National Science Foundation Biological Centers Facility, member of the editorial advisory board of the journal *Analytical Chemistry*, and chairperson of the East Tennessee Mass Spectrometry Discussion Group.

Gary Glish has been elected vice president of the American Society for Mass Spectrometry.

Barry Berven has been named associate division director of ORNL's Health and Safety Research Division. He also is president-elect of the Oak Ridge Chapter of Sigma Xi and of the Environmental Section of the Health Physics Society.

The following researchers in ORNL's Fusion Energy Division have been elected fellows of the American Nuclear Society: **Charles C. Baker, Paul N. Haubenreich,** and **Nermin A. Uckan**.

The following researchers in ORNL's Fusion Energy Division have been elected fellows of the American Physical Society: **Lee A. Berry, Benjamin A. Carreras, R. A. Dory, Julian L. Dunlap, David W. Swain,** and **John H. Whealton**.

F. Owen Hoffman has been selected by the governor of Colorado to serve on an advisory panel assessing possible health risks at DOE's Rocky Flats Plant. He also has been appointed to the Hanford Thyroid Morbidity Study Advisory Committee of the Centers for Disease Control by the Secretary of the U. S. Department of Health and Human Services.

Lowell Langford has been named Energy Systems' technical information officer, and **Rebecca A. Lawson** has been named ORNL site records manager.

T. S. (Tom) Kress has been named head of the Applied Systems Technology Section of ORNL's Engineering Technology Division.

For the third time in the past four years, **Stan David, John Vitek,** and **Allison Baldwin** have received the International Metallographic Society's Pierre Jacquet Gold Medal and the Lucas Award of ASM International, the grand prizes in a major international metallography competition. The two awards recognize a technical poster entered in the international competition's electron microscopy category entitled "Controlled Residual Elements Improve Creep Properties of Stainless Steel Welds."

Lee R. Shugart has been named director of the NATO Advanced Research Workshop on Strategy for Biomarker Research and Application in the Assessment of Environmental Health.

William R. Hamel has been reappointed to the U.S. Army Science Board.

Bill Cabage has been named editor of *Lab Notes*, ORNL's newsletter.

Roger A. Jenkins has been elected to the editorial board of *The Journal of Smoking-Related Disorders*.

J. Michael Ramsey has been elected chairman of the program committee of the

Division of Analytical Chemistry of the American Chemical Society.

W. D. Shults is chairman-elect of the East Tennessee Section of the American Chemical Society.

Marcus B. Wise has been elected chairman of the Environmental Interest Group of the American Society for Mass Spectrometry.

Yousrey Y. Azmy has been elected treasurer of the Mathematics and Computations Division of the American Nuclear Society.

Daniel T. Ingersoll has been elected chairman of the Radiation Protection and Shielding Division of the American Nuclear Society.

Robert T. Santoro has been elected to the executive committee of the Radiation Protection and Shielding Division of the American Nuclear Society.

Mark S. Smith has been elected to the executive committee of the Oak Ridge/ Knoxville Section of the American Nuclear Society.

François G. Pin has been elected program chairman of the Robotics and Intelligent Interfaces Third International Conference for Industrial and Engineering Applications of AI and Expert Systems. He also has been named to the editorial board of the *International Journal of Robotics and Mechatronics* and the *Journal of Advanced Automation Technology*, published in Japan. He is now guest editor of the *Computers and Electrical Engineering Journal.*

R. J. Carter has been elected editor of the *Human Factors Society Bulletin.*

Everett E. Bloom has been appointed a member of the International Advisory Committee of the International Conference on Physics of Irradiation Effects on Metals.

Stan David has been appointed chairman of the Joining Division Council of ASM International and member of the nominating committee of ASM International.

James R. Keiser has been appointed secretary for the energy technology committee of the National Association of Corrosion Engineers.

Louis K. Mansur received a 1990 DOE Materials Sciences Research Competition Award for Significant Implications for DOE-Related Technologies for his work in explaining early reactor wall embrittlement in terms of "enhanced point defect survival." He also has been named editor of the *Journal of Nuclear Materials.*

Stephen J. Pennycook has received the 1990 DOE Division of Materials Science Award for Outstanding Scientific Accomplishment in Solid State Physics.

Gerald M. Slaughter has been elected a fellow of the American Society for Nondestructive Testing and a fellow of the American Welding Society.

Richard J. Olson is helping the President's Council on Environmental Quality design a more comprehensive program to report on environmental trends.

Peter F. Tortorelli has been elected chairman of the Oak Ridge Chapter of ASM International.

M. H. Yoo received an award in the Metallographic Photo Contest of the Japan Institute of Metals.

F. M. Martin has been elected councilor of the Southeast Chapter of the Society of Toxicology.

Jerry D. Garrett has been elected chairman of the 1991 Gordon Research Conference on Nuclear Chemistry.

Ronald A. Phaneuf has been elected to the Committee on Atomic, Molecular, and Optical Science of the National Research Council.

Gerald D. Mahan has been elected member-at-large of the Executive Committee of the Division of Condensed Matter Physics of the American Physical Society.

Larry W. Barnthouse has been appointed to the National Research Council's Committee on Risk Assessment Methodology and was chairman for the Council's Workshop on Ecological Risk Assessment, held recently in Warrenton, Virginia.

John C. Glowienka, former operations manager for

Lou Mansur

Dick Olson

Larry Barnthouse

Melvin Feldman

Monica Turner

Fran Sharples

Karen Von Damm

the Advanced Toroidal Facility in ORNL's Fusion Energy Division, has been named head of the Operational Readiness Section of ORNL's Office of Operational Readiness and Safety.

Melvin J. Feldman has received the Ray Goertz Award from the American Nuclear Society in recognition of his "outstanding contributions to the advancement, application, and utilization of remote technology in the nuclear industry."

J. R. Noonan has been elected to the Board of Directors of the American Vacuum Society.

C. Woodrow White has been elected co-chairman of the Seventh International Conference on Ion Beam Modification of Materials.

Monica G. Turner has been appointed a member of the Directorate for Temperate Ecosystems for the U. S. National Committee for the Man and the Biosphere Program. She also has been named an editorial advisor to *Climate Research*, a new international scientific journal.

Glenn W. Suter II has been elected a member of the board of directors of the Society of Environmental Toxicology and Chemistry.

Frances E. Sharples has been appointed a member of the Committee on Science, Engineering, and Public Policy of the American Association for the Advancement of Science.

Keith Eckerman has been elected a member of the National Council on Radiation Protection and Measurements.

David E. Reichle has been elected a member of the Board of Council of the International Union of Radioecologists.

Steven F. Railsback has been awarded the Antarctica Service Award of the United States of America by the National Science Foundation and the Department of the Navy for service in Antarctica. He participated in developing an environmental impact statement for all activities of the U. S. Antarctica Program.

Kowetha Davidson and **Bob Young** recently were certified by the American Board of Toxicology.

Patrick J. Mulholland has been named to the editorial boards for the journals *Ecology* and *Ecological Monographs.*

Karen L. Von Damm has been appointed a member of the Alvin Review Committee of the University–National Oceanographic Laboratory System. The *Alvin* is the main submersible used by the U.S. scientific community for oceanographic research.

Glenn F. Cada has been elected a fellow of the American Institute of Fishery Research Biologists.

Carolyn T. Hunsaker has been named a consultant to the Ecoregions Subcommittee of the Science Advisory Board of the U. S. Environmental Protection Agency.

Stephen H. Stow has been named chairman of the international Commission on the Hydrogeology of Hazardous Wastes.

Philip S. Sklad has been elected a director of the Executive Council of the Electron Microscopy of America.

Thomas S. Kress has been appointed head of the Applied Systems Technology Section of ORNL's Engineering Technology Division.

RE: Pick a Number

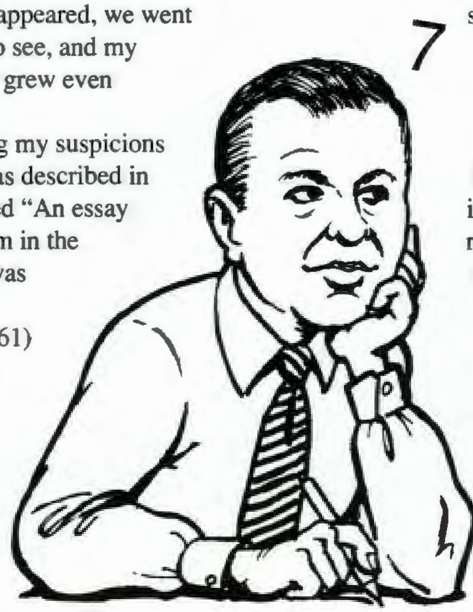
Improving Hunches and the Bayes Formula

By Alan Solomon

Recently my son and I differed over which movie to see. With a sly look, he took a coin from his pocket and suggested that we base our decision on whether "heads" or "tails" came up on a toss. "If it's heads," he said, "we'll see my movie. If it's tails, we'll see yours."

When I inquired jokingly if his coin were two-headed, he appeared overly shocked that I had asked such a question. His response aroused my suspicions, but I did not demand to see his coin. He tossed it, heads appeared, we went to the movie he wanted to see, and my suspicions about his coin grew even stronger.

A means for expressing my suspicions in mathematical terms was described in a 1763 publication entitled "An essay towards solving a problem in the doctrine of chances." It was written by the Reverend Thomas Bayes (1702–1761) and published two years after he died. The key contribution of this work is the Bayes formula, a relation that can be used to improve initial predictions about the likelihood that a certain event will occur—"prior probability"—on the basis of additional evidence collected later. An improved probability is called a "posterior."



In the case of my son's coin toss, a prior belief (before the toss) that the coin has a 10% chance of being two-headed, would be raised to 18% after the toss, and a prior probability of 50% would lead to a posterior probability of 67%.

Although the Bayes formula appears to be reasonable, it has aroused controversy about the fundamental concept of probability—namely, whether the probability of an event happening can be found only after many experiments (e.g., coin tosses) or whether it is simply the "odds" that may be corrected in time and that might be based partly or only on intuition (e.g., the sneaky look in my son's eye).

The latter approach, which is based on revising an initial guess about the probability of the coin having two heads after a coin toss yields a head, has led to the use of the Bayes formula in such areas as decision making in robotics, data collection in waste management, and expert systems (e.g., in medical diagnosis). A more familiar application is the computerized election-night prediction whose accuracy improves as votes are counted.

More philosophically, this approach enables us to bridge a gap between pure intuition and the quantification of inexact knowledge in a useful way. Of course, it also makes possible a lack of faith in "honest" coin tosses!

A precise formulation and derivation of the Bayes formula is found in most books on probability and statistics. *Probability and Statistics* by Morris DeGroot (Addison-Wesley, 1975) is one of my favorites.

Editor's Note—The ORNL Review *has a new mathematics columnist succeeding Ram Uppuluri, who retired in 1990. Alan David Solomon is an ORNL consultant who served as a group leader in the Mathematics and Statistics Section of ORNL's Engineering Physics and Mathematics Division. A resident of Israel who has a Ph.D. degree in mathematics from New York University, Solomon has experience in applied mathematics, energy and energy storage, phase change processes, and robotics and artificial intelligence. He is currently working in motor current signature analysis, optimal control of thermal energy storage systems, and in situ bioremediation of chemical wastes.*

Science in Action

"This is going to be the worst 45 minutes of your life."

A student who works at the Clinch River Raptor Center takes Rusty, a screech owl, out to visit with students during a presentation at Science in Action in Knoxville. The program made science exciting for hundreds of students.

You know the stereotypes. A lot of people, especially middle and high school students, believe that science is boring and that scientists are especially boring.

But Science in Action exploded that myth. First a group of middle school students presented a program on raptors, complete with wildlife magazine–quality slides and owls who were walked through the audience, that left the crowd full of questions and enthusiasm. Then Michael O'Hern blew into the room with a barrage of razzle-dazzle showmanship and kid-oriented patter that still taught a lot about the basics of materials sciences. The students left convinced that science is not just the realm for geeks and nerds.

Science in Action was held for the second year as a part of the 1991 WATTec, the annual Knoxville conference for scientists and engineers. The program ran for four days and brought in students from 30 elementary, 9 middle, and 15 high schools. Cosponsored by ORNL, the Aluminum Company of America, and the Tennessee Valley Authority, the program covered subjects from natural history to mathematics and statistics.

Two ORNL researchers, Linda Horton of the Metals and Ceramics (M&C) Division and Julie Watts of the Environmental Sciences Division, worked to develop and carry out the program. "An important outgrowth of the program has been that the schools now know what we have to offer," said Watts. "The East Tennessee Discovery Center has a traveling trunk that goes to all elementary schools as a part of the Science in Action program, and the trunk is now booked through the end of the school year. And the teachers are calling ORNL to have science programs brought into their classrooms. Science in Action is a really successful program that reaches a lot of different schools."

When Peter Tortorelli, also of ORNL's M&C Division, welcomed the students, he said, "Some of us believe that this is the most important aspect of

"Some of us believe that this is the most important aspect of WATTec—reaching out to students with science and mathematics."

WATTec—reaching out to students with science and mathematics."

The Clinch River Raptor Center, a Clinton Middle School program created by a science teacher, opened the February 21 program with often enchanting photographs of the birds that the staff rescue, heal, and return to the wild. The slides were narrated by three middle school students who obviously "knew their stuff" and loved the work they did. By the end of the presentation, the audience knew that raptors are birds of prey.

After the slide show, the Raptor Center students brought two owls from their boxes and walked them through the crowd. A red-tailed hawk kept trying to fly clear from the gloved hand of one student, so she was kept at the front of the room. The fascinated students had a lot of questions: "How many mice does she eat a day?" "Where was she found?" "What kind of gun was she shot with?" "Have you ever gotten the same bird twice?" "Do you ever turn them loose?" "How many do you release in a year?" Persuading the most uncooperative hawk back into her box added a note of danger to the presentation.

The students were then broken into four small groups of about thirty for the next presentations. When "Fun with Materials" began, it was clear that it would be fun indeed.

Michael O'Hern, a former member of the M&C Division, strode in and asked, "What in the world is going on in here?" As he set up his equipment, he joked with and questioned the students. He promised that "this is going to be the worst 45 minutes of your life." He was intense, he was funny, and he wanted the students to be involved in this learning session.

"What is this?" asked the students when they were handed metal disks about the size of a quarter.

"Examine it!" thundered O'Hern.

And under O'Hern's tutelage they learned that the disks contain metal crystals. They learned the three phases of matter, the three types of solids (metals, polymers, and ceramics), and the characteristics of these solids. They learned why a marching band is like a crystal—the members of the band are aligned in neat rows, as are the atoms in a crystal. They saw tin melted, frozen, and spun into showers of tinsel. They found out that this tinsel tin is no longer crystalline. And they had a good time.

O'Hern even worked in a safety statement. As he put safety glasses on a volunteer for a demonstration, he turned to the crowd and said, "Does he look like a geek?"

"Yes!" chorused the crowd.

Seriously, O'Hern said, "I would rather look like a geek than never be able to see another geek in my life. Always wear safety glasses to protect your eyes when you're doing an experiment."

O'Hern closed his presentation with "OK, so who really gives a rip about materials? You don't need to, because you'll certainly never use a computer. And you'll probably never want to buy a car. And you'll certainly never fly in an airplane." He explained that materials are a part of what we buy and use every day.

These sorts of demonstrations make students clamor to volunteer and encourage questions and interaction. Science in Action moves the students to action. Mr. Wizard is not alone.
—*Cindy Robinson*

ORNL Researchers Win Gordon Bell Prize for Scientific Computing

Malcolm Stocks (left) of the Metals and Ceramics Division and Al Geist of the Engineering Physics and Mathematics Division shared the Gordon Bell Prize for price/ performance in scientific computing. They used special computer codes on the new Intel parallel processor at ORNL to model the electronic structure of a high-temperature superconductor (shown as stick model).

A team of researchers at ORNL has won the 1990 Gordon Bell Prize for superior effort in price/ performance in scientific computing.

Al Geist of ORNL's Engineering Physics and Mathematics Division, Malcolm Stocks of ORNL's Metals and Ceramics Division, Benjamino Ginatempo, a visiting faculty member from the University of Messina in Italy, and Bill Shelton, a former Oak Ridge Associated Universities postdoctoral fellow, now at the Naval Research Laboratory, made up the winning team. The team received the prize for their calculations of the electronic structure of a high-temperature superconductor on parallel computers at ORNL.

The announcement of prize winners was made February 27 at the IEEE Compcon Conference in San Francisco. The conference is sponsored by the Institute of Electrical and Electronic Engineers, Inc. (IEEE), which administers the awards.

The Gordon Bell Prize was established in 1987 to recognize significant achievements in the application of supercomputers to scientific and engineering problems. This year the main prize was given out in the category of price/ performance. Lesser awards were also presented in the categories of compiler parallelization and performance.

Gordon Bell, who puts up the funds for the prize, is well known in the computer industry and has had a distinguished career in computer design and architecture. One of his most notable accomplishments was the design of the popular Digital Equipment Corporation VAX computer. He now works as a computer consultant.

ORNL's winning entry was cited for three major accomplishments. First, the researchers achieved a computation rate of 2.5 gigaflops (billion floating point operations per second) using the Intel iPSC/ 860 computer at ORNL. This is the first application program in the world to exceed 2 gigaflops on this type of parallel computer.

Second, again using the Intel computer, the researchers achieved a price/performance ratio of 840 megaflops (million floating point operations per second) per $1 million (based on the list price of the computers used). This ratio is over two times higher than last year's winning entry.

Third, the researchers' winning price/performance ratio of 2000 megaflops per $1 million was achieved using a network of IBM RS/6000 workstations and a software package called PVM (Parallel Virtual Machine) developed at ORNL by Vaidy Sunderam, a visiting faculty member from

Emory University, and Geist. The PVM package allows parallel programs to use all the computers hooked together by a network to solve a single problem.

"We at ORNL are excited about the power of parallel computing and are beginning computations to address unanswered questions in materials science," said Geist, who works in ORNL's Mathematical Sciences Section. The Intel computer allows scientists to perform in a few hours complex calculations that previously required weeks. The research team has been using this computer in their studies of disordered materials. Such disorder results from the substitution of one type of atom in a material by another type, as in the process of alloying.

"Disordered materials include high-temperature superconductors, metallic alloys, magnets, and many other important materials," said Stocks. "The calculation of the electronic properties and energetics of disordered materials could aid scientists in understanding the behavior of these materials."

The ORNL team was studying the electronic structure of a superconductor containing barium, potassium, bismuth, and oxygen when they submitted their entry. These calculations will help theorists better understand the structure of this class of high-temperature superconductor.

Superconductors are capable of conducting current with zero energy loss. Until 1986 it was necessary to cool materials to near absolute zero (–273°C) before they became superconducting. Now scientists have discovered materials that become superconducting at much higher temperatures, but they do not understand why this happens.

Theorists determine the basic properties of materials by considering the identity and concentrations of atoms making up a material and then calculating the forces that bind atoms together. These complex forces act between the positively charged nuclei and the negatively charged electrons that are constantly moving around and between nuclei.

Besides calculations on materials properties, the Intel machine is also being used for other ORNL "grand challenge" problems, such as global climate modeling, gene sequencing, atomic physics, plasma physics, and some computationally intensive problems from other organizations, such as the Superconducting Super Collider Laboratory in Texas.

Architect-Engineer Chosen To Design ANS Facility

Gilbert Commonwealth, Inc., an architect-engineering firm in Reading, Pennsylvania, has been selected to design the facility incorporating the Advanced Neutron Source (ANS), a new research reactor that DOE may decide to build at ORNL.

The firm was chosen by Energy Systems for negotiation of the scope and cost of a contract for the conceptual design of the "balance of plant" of the ANS Facility, which includes the nonreactor part of the facility as well as the reactor cooling system and structures. ORNL will be responsible for the conceptual design of the reactor core, refueling equipment, the reflector tank systems, the reactor control systems, and the experimental systems equipment.

The contract, which will cover a working period of about 15 months, may be in place by the end of the summer, according to ANS Project Director Colin West. Under the contract, Gilbert Commonwealth will be supported by AECL Technologies in Rockville, Maryland; Air Products and Chemicals, Inc., in Allentown, Pennsylvania; DRS/Hundley, Kling, Gmitter in Pittsburgh, Pennsylvania; Geotek Engineering Company in Knoxville; and the University of Tennessee at Knoxville.

The ANS is being considered by DOE as a replacement for aging reactors. As a user facility, it would draw scientists from all over the world. It would be equipped with advanced instruments for neutron scattering and nuclear physics research, and it would provide capabilities for isotope production and the study of materials in high radiation fields.

According to West, "The ANS would put ORNL—and the United States—back in the forefront of scientific research using neutrons."

"The ANS would put ORNL—and the United States—back in the forefront of scientific research using neutrons."

Health Physics Reactor Closed

ORNL's Health Physics Research Reactor (HPRR) has been permanently shut down as a result of an October 18, 1990, order from the Department of Energy. The reason given for the closure is the lack of funds to support reactor restart and research.

The reactor was one of four ORNL reactors shut down in March 1987, about four months after the operation of the High Flux Isotope Reactor was indefinitely suspended because of embrittlement in the wall of the pressure vessel. The HFIR was restarted in January 1990 and brought to full power in May.

Of the four reactors shut down in March 1987, only the Tower Shielding Reactor has been restarted. The Bulk Shielding Reactor awaits a decision on restart. Besides the HPRR, the Oak Ridge Research Reactor was also shut down permanently.

The HPRR had been used for training in radiation dosimetry, radiobiology studies to determine the health effects of radiation on animals, studies for calibrating personnel dosimeters for measuring radiation exposure, and simulations of human-body radiation exposure under normal and accident conditions for guiding the establishment of international limits for radiation exposure.

ORNL Helps Develop New Agent to Study Bone Pain Treatment

Some cancer patients experience bone pain as a result of cancer cells spreading to the skeletal system from a primary tumor, usually in the ovaries or prostate gland. To relieve bone pain in cancer patients, physicians seek radioactive agents that concentrate strongly in the bone and kill the culprit cancer cells.

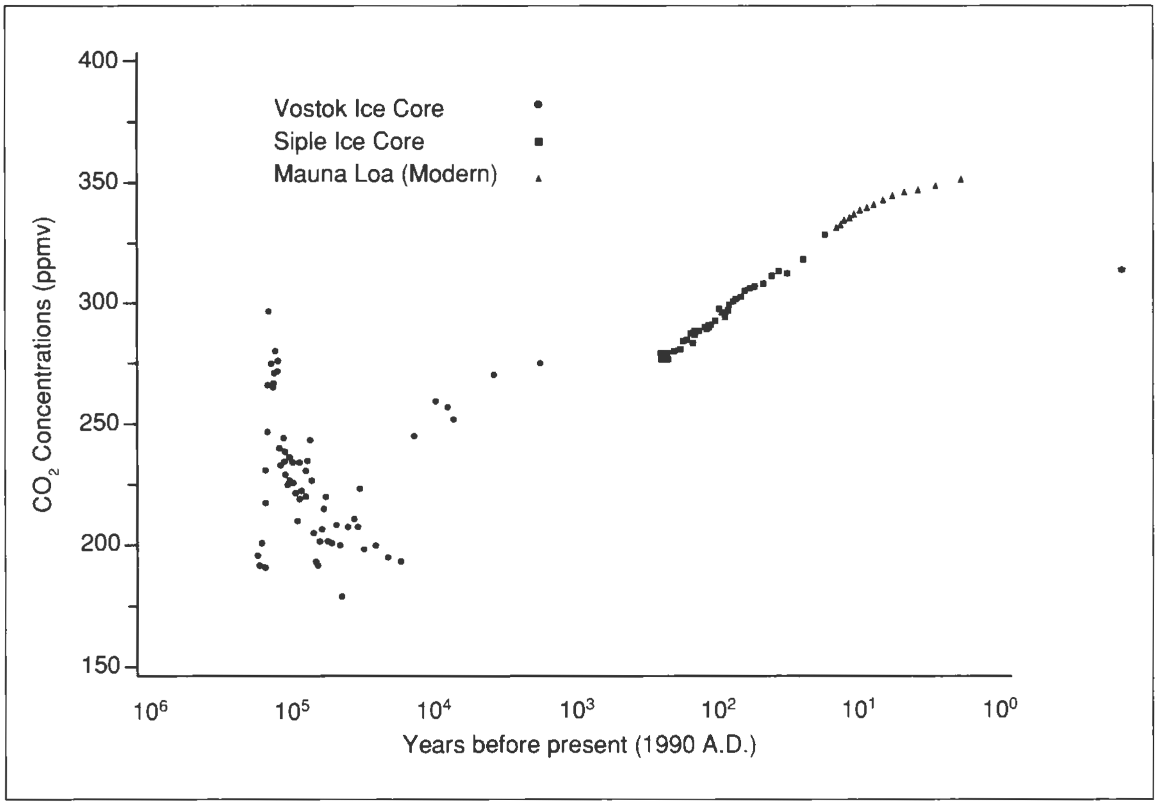
Recent studies of experimental animals by investigators at the Medical Department of Brookhaven National Laboratory (BNL) and at the State University of New York at Stony Brook have shown very high bone uptake of a compound containing radioactive tin. This agent, diethylenetriamminepentaacetic acid (tin-117*m*-DTPA), was prepared from tin-117*m*, which was produced in the HFIR.

With the restart of the HFIR for routine production of radioisotopes, ORNL's Nuclear Medicine Group in the Health and Safety Research Division has reinitiated its collaboration with BNL and Stony Brook researchers. The three groups are now conducting the first patient studies using tin-117*m*-DTPA for treatments to relieve bone pain in cancer patients.

In the early 1980s, the Nuclear Medicine Group was investigating new tin-117*m* -labeled radiopharmaceuticals and developed an efficient technique to prepare metallic tin-117*m* from tin-117*m*–tin dioxide produced by irradiating a tin dioxide target enriched in tin-116 with neutrons from the HFIR. From 1983 through 1985, the tin-117*m* was chemically processed at ORNL and was sent to BNL for preparation and testing of the tin-117*m*-DTPA.

The BNL researchers in this collaborative study found that tin-117*m*-DTPA (1) concentrates strongly in cortical bone, depositing radiation there with minimal radiation dose to the bone marrow (the key to the immune system), and (2) delivers a high enough radiation dose (up to 21 rad/mCi) to make tin-117*m*-DTPA a good candidate for treatment of cancer-related bone pain in humans.

For the initial patient studies that will be conducted at the Department of Nuclear Medicine at Stony Brook in conjunction with BNL investigators, ORNL researchers are now using the HFIR to irradiate tin-117, rather than tin-116, to produce tin-117*m*. The product is shipped to BNL for preparation of the agent.



This graph showing the annual atmospheric CO_2 concentrations during the past 160,000 years (derived from the Vostok and Siple ice cores and Charles Keeling's Mauna Loa record) appears in *Trends '90.*

In the first phase of the patient studies at BNL, tracer levels of the tin-117*m*-DTPA will be administered to cancer patient volunteers. Gamma camera imaging will be used to determine if bone uptake of tin-117*m*-DTPA is high in humans. Results of the initial studies will guide additional therapeutic studies planned at Stony Brook.

ORNL Publishes Global Change Data Book

ORNL has published a detailed summary of data on changes in the global environment. The 250-page report is expected to facilitate exchanges of information among scientists throughout the world and make data more readily available to researchers, science reporters, educators, managers, students, and information specialists. Information provided in this report consolidates a wealth of data scattered throughout the scientific literature.

Called *Trends '90: A Compendium of Data on Global Change*, the one-volume publication is a unique collection of information on atmospheric carbon dioxide (CO_2) and methane concentrations dating back 160,000 years; assessments of worldwide and national trends in CO_2 emissions from fossil fuels; and long-term global, hemispheric, and regional temperature records.

The report was written by Tom Boden, Mike Farrell, and Paul Kanciruk, all of the Carbon Dioxide Information Analysis Center (CDIAC) at ORNL. Its information should be useful to scientists trying to predict possible climate effects from increased atmospheric concentrations of carbon dioxide, methane, and other greenhouse gases resulting from energy production and other sources. Global warming could be induced by an intensified greenhouse effect in which elevated concentrations of greenhouse gases increasingly block the release of heat from Earth's surface, causing the surface air temperature to rise. Such a global warming is of concern to policymakers because of potentially disruptive environmental and socioeconomic effects.

About 60 scientists worldwide provided ORNL with data collected from scores of sampling sites. Boden, lead author of the report and information specialist in ORNL's CDIAC, states that the document was made possible by "the willingness of these researchers to make their data available to a larger audience of national and international scientists, students, and policymakers." Farrell, a coauthor of the report and head of the the Earth Systems Section of ORNL's Environmental Sciences Division, added that the data in the report have "undergone extensive checks to ensure accuracy and have been carefully documented by CDIAC staff."

According to Kanciruk, "Each two-page presentation of the report is a condensation of reams of information. Ten pages of information is often distilled into a paragraph or two. This intermediate level of reference will save people valuable time by eliminating the need for extensive searches of other scientific literature."

One section contains precise records of past and present atmospheric concentrations of CO_2 needed for modeling and understanding the global carbon cycle and possible CO_2-induced climate change. An important source of information about past concentrations has been the analysis of Antarctic ice cores.

Another section presents information about global and national CO_2 emissions from fossil fuel burning, cement production, and gas flaring. The data show that in 1988 the United States, the Soviet Union, and the People's Republic of China were responsible for over half of the world's CO_2 emissions from fossil fuel burning.

The report also presents data on atmospheric concentrations of methane, which is produced by coal mining, natural gas production and distribution, oil exploration and production, biomass burning, fermentation, and other sources. Information on past atmospheric methane concentrations has been obtained by analyzing air bubbles in ice from Greenland and Antarctica. Studies under way since 1978 indicate that atmospheric methane concentrations have risen 1 to 2% per year.

The section on temperature records describes temperature trends as far back as the 1860s. Measurements of surface air temperatures show a warming trend, particularly in the 1980s, but the ORNL report states that it is unclear whether these trends result from a buildup of greenhouse gases or from other factors, such as the greater frequency of El Niño/Southern Oscillation events in the Pacific Ocean.

Data from *Trends '90* have been cited in several federal reports, including *America's Climate Change Strategy: An Action Agenda*, produced by the Executive Office of the President of the United States. The versatility of *Trends '90* is demonstrated by its selection as a textbook for the graduate course "Earth Systems Education," which was taught at Ohio State University in the spring of 1991.

All data in *Trends '90* are available in digital form from the Carbon Dioxide Information Analysis Center.

Changes in ORNL's Work for the SSC

The Oak Ridge Detector Center will be involved in three detector development projects for the Superconducting Super Collider (SSC).

According to Tony Gabriel, director of the Detector Center, ORNL researchers will be working with the Solenoidal Detector collaboration led by George Trilling of DOE's Lawrence Berkeley Laboratory and with the Super Fixed Target collaboration directed by Brad Cox of the University of Virginia.

In addition, ORNL is involved in a new collaboration to build a second large detector to replace the proposed L* detector, which the SSC Laboratory rejected in May 1991. The new effort, which is being encouraged by the SSC Laboratory, is led by Bill Willis of Columbia University and Barry Barish of the California Institute of Technology.

The Detector Center will be developing the central tracking system for the only large detector approved for the SSC—the Solenoidal Detector. This system will track the directions and measure the initial energies of the first particles produced when the two opposing beams of protons collide in the oval track of the SSC accelerator, to be built by 1998 in Waxahatchie, Texas. ORNL personnel also will support the development of the smaller Super Fixed Target detector, which will determine the characteristics of the "bottom quark," a building block of subatomic particles.

Frank Plasil of the Physics Division is ORNL's representative on the Collaboration Council for the proposed second large detector. He says that the Council is pushing for a detector that will complement the general-purpose Solenoidal Detector by specifically measuring very accurately the energies of electrons, photons, and muons produced in proton-proton collisions. ORNL's involvement with the collaboration will probably deal with calorimeters, devices within the detector that determine the energies of electrons, photons, and hadrons (e.g., protons and neutrons).

ORNL's strength in basic high-energy physics research is increasing as a result of efforts by Plasil, ORNL Director Alvin Trivelpiece, and others to build a group of experts in particle physics. Ken Reed, a high-energy physicist, has joined the Physics Division as a collaborative researcher with ORNL and the University of Tennessee at Knoxville. In addition, Yuri Kamishkov of the Institute of Experimental and Theoretical Physics in Moscow is now working in the Physics Division for two years; five Soviet scientists have been assigned to collaborate with him for three to six months here on the development of liquid-scintillation calorimetry technology.

ORNL will continue its collaboration with the consortium of universities known as the Southern Association for High Energy Physics (SAHEP). Many of these universities are included in one or more of the collaborations formed to carry out research at the SSC Laboratory. This consortium, chartered under the Oak Ridge Associated Universities, recently received $1 million from the Texas National Laboratory Research Commission for research on and development of computer simulations of proton collisions, energy deposit measurement technology, particle tracking and identification systems, radiation resistance technology, fast detector electronics, and other projects.

The $1 million will be divided among the 20 universities in SAHEP. ORNL will not receive any of the Texas funding because national laboratories are not eligible. The SSC Laboratory is expected to provide DOE funds to support all of the Oak Ridge Detector Center's activities this fiscal year at a level of about $1.6 million, according to Gabriel.

About 12 full-time equivalent persons are associated with the Oak Ridge Detector Center. Gabriel says this number is expected to rise to 25 to 30 in the next two years, about two-thirds of the expected number of personnel if the L* detector proposal had been approved.

ORNL researchers working on these projects come from the Applied Technology, Engineering Physics and Mathematics, Fusion Energy, Health and Safety Research, Instrumentation and Controls, and Physics divisions and the Central Engineering Organization and Computing and Telecommunications Division of Martin Marietta Energy Systems. ornl

Female-Specific Genetic Damage Discovered by ORNL Biologists

Through their studies of fetal mice, Walderico Generoso (right) and Amany Shourbaji have found that some chemical mutagens affect females but not males. ORNL is the only U.S. laboratory conducting systematic studies on the effects of radiation and chemicals on female mice.

Mice show sexual differences in their responses to certain chemicals, according to research conducted by ORNL's Biology Division with funding from the Department of Energy and the National Institute of Environmental Health Sciences. The results suggest that certain anticancer drugs pose genetic risks to women but not to men.

The researchers discovered that certain chemicals are "gender-specific" mutagens because they cause genetic damage only in one sex. In particular, they found that the anticancer drugs adriamycin and platinol cause "dominant-lethal" mutations in the germ cells of female but not of male mice. Dominant-lethal mutations, detectable by the increased death rate of early embryos, result from genetic damage in parental germ cells—the sex cells that pass traits from one generation to the next.

The original discovery involving these chemicals was published by the ORNL researchers in *Mutation Research* in early 1990. Since that time, the ORNL group discovered similar results for hycanthone, a drug used to combat schistosomiasis (a disease of people living in less developed countries, caused by a parasitic worm). The results were published in the January 1991 issue of *Mutation Research.* Similar results, not yet published, were also found for another anticancer drug.

ORNL, well known for decades of studies on the genetic effects of radiations and chemicals in mice, is the only laboratory in the United States conducting systematic studies on females. These experiments are led by Walderico Generoso of the Biology Division.

"Our results," said Generoso, "suggest that therapeutic drugs found to be female-specific mutagens in mice should not be used in women and girls if a safer substitute can be found. However, we recommend that certain of these drugs be used as substitutes for alkylating drugs that damage or kill male germ cells."

In females, oocyte germ cells within ovaries mature into eggs, which are discharged from ovaries; in males, a progression of germ-cell stages mature into sperm. If damage to the chromosomes (carriers of genes) within any of these cells is severe enough, dominant-lethal mutations can result, causing some of the offspring of mated mice to die before birth.

The experiment at ORNL involved mating male mice injected with one of the test drugs with noninjected females and mating injected females with noninjected males. In each case, pregnant mice were opened up surgically, and dead embryos were counted. No increase in dead embryos was found for noninjected female mice mated with injected males—that is, dominant-lethal mutations had not been induced in male germ cells.

However, a significant increase in dead embryos was discovered in female mice that had been injected with one of the chemicals before they were mated to noninjected males. Additional experiments ruled out the possibility that these excess deaths were caused by the chemical's effects on the uterine environment of the embryos, indicating that the deaths resulted from dominant-lethal mutations induced in female germ cells.

The researchers think that the test chemicals break the chromosomes of female, but not male, sex cells because of the special shape and structure of the female chromosomes.

"We believe there are at least two mechanisms that cause genetic damage in female germ cells," says Generoso. "One mechanism is intercalation. Hycanthone and two anticancer drugs that we tested caused damage by inserting, or intercalating, themselves between DNA base pairs in the female germ cells. Because the oocyte chromosomes are more stretched out than those of sperm, the damaging chemicals insert themselves more easily in the female chromosomes.

"A second mechanism may be illustrated by the third anticancer drug we tested. This chemical is thought to bind to DNA bases that are in unique sequences. Such sequences are inaccessible in male germ cells but are accessible in females because of the spread-out nature of their germ-cell chromosomes."

The ORNL group is the first to demonstrate the existence of female-specific chemical mutagens. The findings show that the results of mutagenicity studies in one sex may not always apply to the other sex.

These findings come at a time when the lack of research on women's specific health problems has received considerable attention. Women health activists argue that most government-supported clinical trials involve only male subjects and that only a small amount of support is given to researchers studying health problems affecting women only or primarily, such as breast cancer, osteoporosis, and menopause.

Most laboratories doing mutagenesis research have performed experiments on male animals only. Generoso says there are two reasons for this:

"First, it has been assumed that chemicals that are mutagenic in females will automatically be detected in tests using males. Prior to our experiments, it was true that all test chemicals that produced mutagenic responses in female animals were also mutagenic in males, although not all mutagens that were positive in males were also positive in females.

"Secondly, it is much easier to perform tests in males because there are no complications from nongenetic effects since the males do not bear the offspring. In tests on females, on the other hand, the possibility that embryonic deaths are caused by the chemical's toxicity to the mother, instead of by genetic damage to the germ cells, must be addressed each time, complicating the research procedures."

Generoso's group is part of ORNL's Mammalian Genetics Section, which has a long history of research on male as well as female mice. Studies with ionizing radiation on teratogenic (birth-defect–producing) effects and on genetic effects in female germ cells were published as long ago as the early 1950s by William L. Russell and Liane B. Russell (now head of the section). Since Generoso came to ORNL in 1967, researchers in the section have studied the genetic effects of chemicals on female mice.

The research was conducted by Motoe Katoh, a former postdoctoral fellow at ORNL who is now in Japan; P. D. Sudman, a former postdoctoral fellow at ORNL who is now at Louisiana State University at Baton Rouge; and members of a Biology Division group led by Generoso—Katherine Cain, Lori Hughes, and Lea Foxworth.

Four years ago, a research team led by Generoso found that just-fertilized eggs in female mice are vulnerable to certain mutagenic chemicals, such as ethylene oxide (used to sterilize hospital instruments). The work suggests that pregnant women who don't yet know they are pregnant and who work in potentially hazardous environments may be exposing their just-conceived children to agents that cause birth defects.

X-Ray Analysis of Crystals Allows View of DNA Features

An ORNL researcher has made uniform single crystals of genetic material from chickens and humans, allowing him to use X-ray analysis to view structural features of DNA almost as small as atoms. DNA carries the genetic blueprint of all organisms.

To better understand how DNA structure makes genes work, Gerard J. Bunick, coordinator for structural biology at ORNL and member of ORNL's Biology Division, has made progress in revealing atomic details of a DNA-protein complex. By using X-ray diffraction, he can view the nucleosome—the basic structural unit of the chromosome—at almost an atomic-level resolution.

The nucleosome, a repeating unit of genetic material, consists of a sphere of proteins wrapped with intricately coiled and folded strands of DNA. DNA forms genes, which are located on chromosomes and which make organisms function and pass traits on to the next generation.

"In a nucleosome, eight proteins form a roughly spherical structure," says Bunick. "The DNA strand winds twice around each sphere, like a hose wrapped around a tennis ball, and then continues to the next nucleosome. Our work should pave the way to understanding how the DNA interacts with the protein core and takes on a structure that affects the functioning of living cells."

A major goal of research in human genetics is to identify gene locations on chromosomes and the sequence of DNA bases within those genes. The Human Genome Project is the driving force behind achievement of this goal.

However, understanding how genes work requires knowledge of the mechanism by which they are turned on and off—that is, the way that they express or fail to express the messages in the genetic code. Such expression is believed to be affected not only by the sequence of DNA bases but also by the three-dimensional structure of nucleosomes.

To see smaller details, Bunick has made uniform nucleosomes, which are then crystallized by varying the metal ion concentration in a solution. To determine the structure of the nucleosome crystals, he is using X-ray diffraction analysis.

In X-ray diffraction, X rays are passed through the crystal, producing a diffraction pattern based on varying concentrations of electrons in the crystal that provides information about its structure. Using baseline information and computing techniques, researchers will calculate the distribution of electron densities in the nucleosome to a resolution of 3.5 Å, or near-atomic resolution.

Several years ago, using nonuniform nucleosomes having heterogeneous DNA strands, Bunick obtained X-ray diffraction measurements at a resolution half as good, or about 8 Å. Using these results, he produced a three-dimensional electron density map and a colored, computer-generated representation of the nucleosome structure.

Nucleosome crystals show an array of color under polarized light (see color photo on back cover). Bunick made these crystals of basic structural units of chromosomes formed from a spherical core of eight proteins (from chicken red blood cells) and wrapped with a human DNA strand that positions precisely and reproducibly on the protein core and that has a known sequence of DNA bases. Because of the way these nucleosomes were reconstituted, the fine details of crystal structure can be determined by X-ray diffraction at a resolution of 3.5 Å, which is close to the sizes of and distances between atoms. The near-atomic resolution of diffraction should provide detailed information on DNA structure and the interactions between protein and DNA.

To make the uniform nucleosomes necessary for a high-resolution view of DNA structure, Bunick isolated the eight-protein spherical cores from chicken red blood cells by using a bacterial enzyme to digest chromatin, the material making up chromosomes. Then he used chemical means to wrap the protein cores with identical segments of human DNA—that is, all DNA strands wrapped around these cores had the same length and the same known sequence of DNA bases. The DNA segments were also positioned the same, so that the sequence of DNA bases were located identically with respect to the individual core histories of each nucleosome.

SERS Technology Licensed to GAMMA-METRICS

The newly licensed SERS is a powerful analytical technique that can be used for environmental monitoring and pollutant control. It was developed by Tuan Vo-Dinh (left) of ORNL's Health and Safety Research Division (HASRD). With him are, from left, Jean-Pierre Alarie, David Stokes, and Gordon Miller, a HASRD staff member. Alarie and Stokes are HASRD contractors.

Energy Systems has licensed a new ORNL-developed continuous monitoring technique to GAMMA-METRICS of San Diego, California, for measuring concentrations of chemical contaminants and other pollutants in water, soil, and wastes.

The new technology is the surface-enhanced Raman scattering (SERS) technique, which uses laser light and layers of organic molecules adsorbed to a silver-coated surface to provide continuous and almost instant measurements of contaminants present in water or some other medium. SERS is a powerful analytical technique that can be used for environmental monitoring and pollutant control. For many organic chemicals, SERS is superior to other analytical techniques.

The SERS continuous monitoring technology was developed by Tuan Vo-Dinh of ORNL's Health and Safety Research Division.

Energy Systems granted GAMMA-METRICS the exclusive rights to commercialize the laser-based SERS continuous monitoring technology to perform real-time, in situ chemical analysis. The company will use the technology initially to measure concentrations of toxic chemicals for site assessments for DOE's Environmental Restoration and Waste Management program.

"The SERS technology extends our analytical and spectroscopic capabilities to the molecular domain," said GAMMA-METRICS president Ernesto Corte. The company plans to build a portable instrument incorporating the SERS technology and make the engineering and other changes needed to accelerate the development and marketing of the analytical technique.

GAMMA-METRICS develops, manufactures, markets, and services instrumentation for diverse industrial applications, such as safety instrumentation for nuclear power plants; pollution control analyzers for the coal industry; analytical instruments and process control for the mining, construction, and environmental industries; and equipment for the high-threat security industries.

The SERS technology is based on the principle that certain organic molecules, when placed on a silver-coated metal surface and excited by laser light, will emit a strongly enhanced light, called surface-enhanced Raman light. If the laser is tuned to emit light of a frequency absorbed by a certain molecule, that molecule will emit Raman light of specific frequencies related to its characteristic vibrations. Detection and measurement of this Raman light allow the identification and measurement of the concentration of the organic molecule in any medium.

Energy Systems Is First DOE Contractor To Sign CRADA

Energy Systems has become the first DOE management contractor to enter into a cooperative research and development agreement (CRADA) established by the National Competitiveness Technology Transfer Act of 1989. The establishment of CRADAs marks a fundamental change in the way the national laboratories interact with industry.

Energy Systems signed a CRADA with an international consortium called the Alternative Fluorocarbons Environmental Acceptability Study (AFEAS). The AFEAS consortium is funded by 12 chemical producers from several countries.

The CRADA enables AFEAS to work with ORNL to study the potential environmental, health, and safety effects of chemicals proposed as alternatives to chlorofluorocarbons to protect the stratospheric ozone layer that protects us from damaging ultraviolet radiation from the sun.

AFEAS will provide two-thirds of the $600,000 cost of the study, with the remainder coming from DOE.

A CRADA is a joint venture between the DOE contractor and industry and provides a means for sharing capabilities, facilities, and technologies available at DOE facilities with U.S. industry, universities, and other research and development organizations for the purpose of improving U.S. competitiveness in the world marketplace.

"A CRADA is a joint venture between the DOE contractor and industry."

"CRADAs provide industry with the opportunity to access the broad R&D capabilities at the DOE facilities," said William Carpenter, vice president for Technology Transfer for Energy Systems. "CRADAs provide a means to bridge the gap between R&D and commercialization."

According to ORNL Director Alvin Trivelpiece, the foundation for CRADAs was laid by the experience of the three DOE high-temperature superconductivity pilot centers, one of which is at ORNL. On August 15, 1990, Energy Systems became the first DOE management contractor to receive authority to implement CRADAs.

Class Patent Waiver in New Contract between DOE and Energy Systems

For many years, the patent rights to any ORNL invention were initially owned by the Department of Energy, making it very difficult to transfer patent rights to industry. In 1984 when Martin Marietta Energy Systems, Inc., was granted the contract to operate ORNL and other facilities for DOE, Energy Systems was given the right to petition DOE for patent ownership rights on a case-by-case basis. Since that time, Energy Systems has petitioned DOE many times for individual patent transfers. Rights to 91 Oak Ridge technologies were obtained, including those transferred to industry through 54 licensing agreements. Under the new contract, 41 pending waivers were automatically approved.

In March 1991, with the renewal of the DOE–Energy Systems contract for another five years, this situation was taken a step further in the interest of expediting technology transfer. DOE granted a class patent waiver to Energy Systems as part of the new contract for the management of the agency's Oak Ridge facilities. Under this novel arrangement, Energy Systems will retain title to most Oak Ridge inventions as they arise. Exceptions include technologies for defense-related applications, uranium enrichment, and the storage and disposal of high-level nuclear waste or spent nuclear fuels.

According to Bill Carpenter, Energy Systems vice president for Technology Transfer, "The class waiver will eliminate a substantial front-end administrative burden for both Energy Systems and DOE. All Energy Systems has to do is to notify DOE that it wants patent rights to a certain invention and then those rights will become the property of the company. This approach will streamline the licensing process and should give a significant boost to our technology transfer program in Oak Ridge. We anticipate a substantial reduction in the time required to get technologies to the marketplace."

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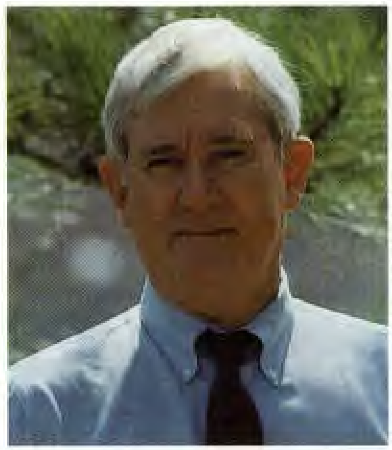

NEXT ISSUE

ORNL Director Alvin Trivelpiece's second State of the Laboratory address tells about ORNL's achievements in meeting DOE's goals in advancing science education and complying with environmental, safety, and health regulations.

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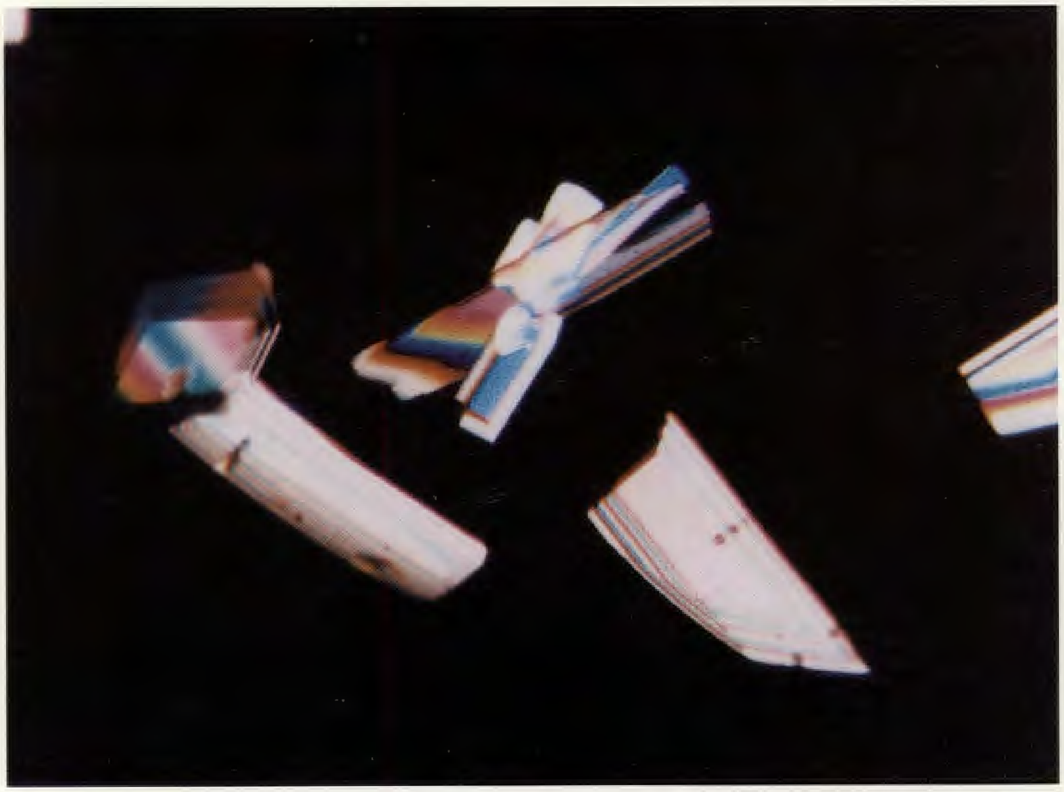

Crystals of nucleosomes (repeating units of chromosomes) are shown under polarized light—the only way they can be made visible. Gerard J. Bunick, coordinator for structural biology at ORNL, made uniform single crystals of nucleosomes using genetic material from chickens and humans, allowing him to use X-ray analysis to view structural features of DNA almost as small as atoms. X-ray analysis of the crystallized DNA winding around the nucleosome's protein core should pave the way to understanding how the DNA interacts with the core and takes on a structure that affects the functioning of living cells. See the description of Bunick's work on p. 60.

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