Oak Ridge National Laboratory

REVIEW

• MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY •

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Delivering *even more* Science

Oak Ridge National Laboratory
REVIEW
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A Higher Expectation

April 1, 2010, was a historic date for Oak Ridge National Laboratory. The day marked not only the tenth anniversary of UT-Battelle's role as the managing contractor for the laboratory, but also the beginning of a new five-year contract announced the previous week at an event attended by Energy Secretary Steve Chu, Tennessee Governor Phil Bredesen, and members of the Tennessee congressional delegation. The announcement was a time to celebrate the accomplishments of the last ten years, mindful that the price of success is a higher level of expectations in the years ahead.

ORNL's message to the Department of Energy and to our stakeholders is a simple one. We view the enormous strides made over the past decade as prologue to what lies ahead. Having transformed an outdated infrastructure into one of the world's most modern research campuses, we are focused in the coming years on using these magnificent facilities to deliver some of the world's most impactful science. Indeed, our belief is that the reputations of the Spallation Neutron Source and the Jaguar supercomputer, along with an array of other exceptional research facilities at ORNL, ultimately will be determined, not by the scale of their extraordinary capabilities, but by the distinction of the science they produce.

This issue of the *Review* is the second of a two-part look at ORNL's efforts to make the laboratory's unique research assets available to a broader segment of the scientific community at other institutions. Our philosophy is predicated on the idea that there is a lasting benefit to the nation in the sharing of research. Approximately 90 percent of the agreements with visiting scientists contain a commitment by the researchers to publish or share the findings of their work at ORNL. We have found this openness frequently enables scientists to build upon the findings of others in their own research projects.

Accessibility to Oak Ridge's user facilities in most cases comes with support from the laboratory's technical and research staff. For many visiting scientists, the willing help and collaboration from ORNL researchers is the "life preserver" that enables them to maximize their time and effort in a new and often intimidating environment. Researchers who arrive in Oak Ridge with preconceived notions on occasion modify their experiments as a result of theoretical calculations or the testing of their materials at ORNL. Equally important, researchers who could perform parts of their research at their home labs often find it more convenient and more productive to conduct the entire experiment while in Oak Ridge.

This commitment by ORNL to "deliver even more science" is the theme not just of this issue of the *Review*, but also of the laboratory's agenda for the next five years. In the same manner as we doubled the size of the laboratory's research program over the last decade, our goal is a comparable increase in the depth and value of the science we deliver to the Department of Energy, to the Congress, and to the public we were created to serve.

Billy Stair
Director
Communications and External Relations

International team discovers element 117

Oak Ridge National Laboratory is part of a team that has added a new chemical element to the Periodic Table. The news came after a paper on the discovery of element 117 had been accepted for publication in *Physical Review Letters*.

The team includes two Russian partners, the Joint Institute of Nuclear Research in Dubna and the Research Institute for Advanced Reactors in Dimitrovgrad. Other team members included Lawrence Livermore National Laboratory, Vanderbilt University and the University of Nevada, Las Vegas.

ORNL's role included production of the berkelium-249 isotope necessary for the target, which was subjected to an extended, months-long run at the heavy ion accelerator facility at Dubna.

"Without the berkelium target, there could have been no experiment," says ORNL Director of Strategic Capabilities Jim Roberto, who is a principal author on the *Physical Review Letters* paper and who helped initiate the experiment.

The berkelium was produced at ORNL's High Flux Isotope Reactor and processed at the adjoining Radiochemical Engineering & Development Laboratory as part of the most recent campaign to produce californium-252, a radioisotope widely used in industry and medicine.

"Russia had proposed this experiment in 2004, but since we had no californium production at the time, we could not supply the berkelium. With the initiation of californium production in 2008, we were able to implement a collaboration," Roberto says.

Roberto worked closely with Yuri Oganessian of Russia's JINR. Five months at the Dubna JINR U400 accelerator's calcium-48 beam—one of the world's most powerful—was dedicated to the project. Lawrence Livermore contributed data analysis, and the entire team was involved in the assessment of the results.

The massive effort produced a total of six atoms of element 117 and the critical reams of data that substantiate their existence.

The two-year experimental campaign began with a 250-day irradiation in HFIR, producing 22 milligrams of berkelium-249, which has a 320-day half-life. The irradiation was followed by 90 days of processing at REDC to separate and purify the berkelium. The berkelium-249 target was prepared at Dimitrovgrad and then bombarded for 150 days at the Dubna facility.

This is the second element that ORNL has had a role in discovering. Element 117 joins element 61, promethium, which was discovered at the Graphite Reactor during the Manhattan project and reported in 1946. ORNL, through the production of radioisotopes for research, has contributed to the discovery of a total of seven new elements.

Members of the ORNL team include the Physics Division's Krzysztof Rykaczewski; Porter Bailey of the Nonreactor Nuclear Facilities Division; and Dennis Benker, Julie Ezold, Curtis Porter and Frank Riley of the Nuclear Science and Technology Division.

Roberto says the success of the element-117 campaign underscores the value of international collaborations in science. "The 117 experiment paired one of the world's leading research reactors—capable of producing the berkelium target material—with the exceptional heavy ion accelerator and detection capabilities at Dubna. This use of ORNL isotopes and Russian accelerators is a tremendous example of the value of working together," he says.

ORNL receives ARPA-E Award

Oak Ridge National Laboratory was among the first organizations to receive funding from the Department of Energy's new Advanced Research Projects Agency-Energy (ARPA-E). The ORNL project is a collaborative effort with Georgia Tech to develop advanced processes and materials that will reduce the cost of capturing carbon dioxide from flue gases, such as those released by power plants. Project scientists are investigating a carbon capture system in which ionic liquids are integrated into novel hollow fiber membranes to form an ionic liquid "sponge" that can absorb carbon dioxide. This technology has the potential to considerably cut the costs and energy associated with capturing carbon dioxide by minimizing the equipment needed, making the technology attractive on a commercial scale.

ARPA-E's first round of awards includes funding for 37 research projects, including almost $1 million for ORNL. ARPA-E's mission is to develop technologies that reduce America's dependence on foreign energy imports, reduce emissions from energy-related processes, improve energy efficiency and ensure that the U.S. plays a leading role in developing and deploying advanced energy technologies.

DOE extends UT-Battelle contract to manage ORNL

The Department of Energy has extended the contract for the University of Tennessee and Battelle Memorial Institute to co-manage Oak Ridge National Laboratory for another five years.

Energy Secretary Steven Chu was joined by Tennessee Governor Phil Bredesen, University of Tennessee Interim President Jan Simek and Battelle President Jeff Wadsworth in announcing the new contract during a visit by Chu to Oak Ridge. UT-Battelle, a joint venture between the two institutions, was first awarded the lab's management contract in April 2000.

"When a lab is being managed as well as Oak Ridge, it makes no sense not to extend the contract," Chu said. "…in this case Oak Ridge was being managed so well there was no need for a competition." The Secretary delivered the news before a group of approximately 350 ORNL and DOE staff.

Since 2000, the state of Tennessee has formed a close relationship with ORNL. Over this period the laboratory has become an increasingly important component of Tennessee's economic development strategy. The recent announcement by a major solar company to locate in Tennessee was credited in part to the opportunity for access to the expertise located in Oak Ridge.

Bredesen's participation in the announcement was evidence of the state's interest in the national laboratory. Bredesen said, "The success of the partnership between UT and Battelle has brought our state world-class expertise in research, high-performance computing, nanotechnology and other areas of science. This announcement ensures Tennessee will be well-positioned to continue to attract research investments and other economic benefits generated by Oak Ridge National Laboratory."

Under UT-Battelle management, the lab has grown from 3,700 to approximately 4,700 employees. During the same period, the laboratory's research portfolio has increased from $640 million to $1.6 billion.

Among the most dramatic changes has been a transformation of an outdated and expensive infrastructure that included dozens of inefficient buildings and miles of chain link fences. With support from the Department of Energy, the state of Tennessee and a creative program of third-party financing, the ORNL campus was rapidly transformed into one of the most attractive and modern research campuses in the DOE laboratory system.

ORNL's modernization included an expansion of science and technology facilities. The most prominent is the $1.4 billion Spallation Neutron Source, completed in 2006 as the world's most powerful pulsed neutron accelerator used in the study the structure of materials at the molecular level.

During UT-Battelle's tenure, Oak Ridge has also become the world's leading center for high-performance computing. ORNL's Jaguar supercomputer, capable of 2,300 trillion calculations per second, is the world's most powerful. UT's Kraken supercomputer, housed at ORNL, is the world's most powerful academic computer and ranks third overall.

Among the most significant developments under UT-Battelle has been the expansion of the partnership between ORNL and the University of Tennessee. Dating back to World War II, the partnership today includes five joint institutes, including four facilities on the ORNL campus dedicated to collaboration in biology, computing, neutron sciences and heavy ion research. The next phase of the partnership will be marked by the creation in 2010 of a new interdisciplinary graduate program in energy and engineering sciences that will include the use of ORNL research staff as UT faculty. The University's partnership with ORNL today includes approximately 60 faculty members with joint appointments and more than 100 students working at the lab. UT and lab officials expect that number to grow to more than 200 faculty and 500 graduate students with the new program.

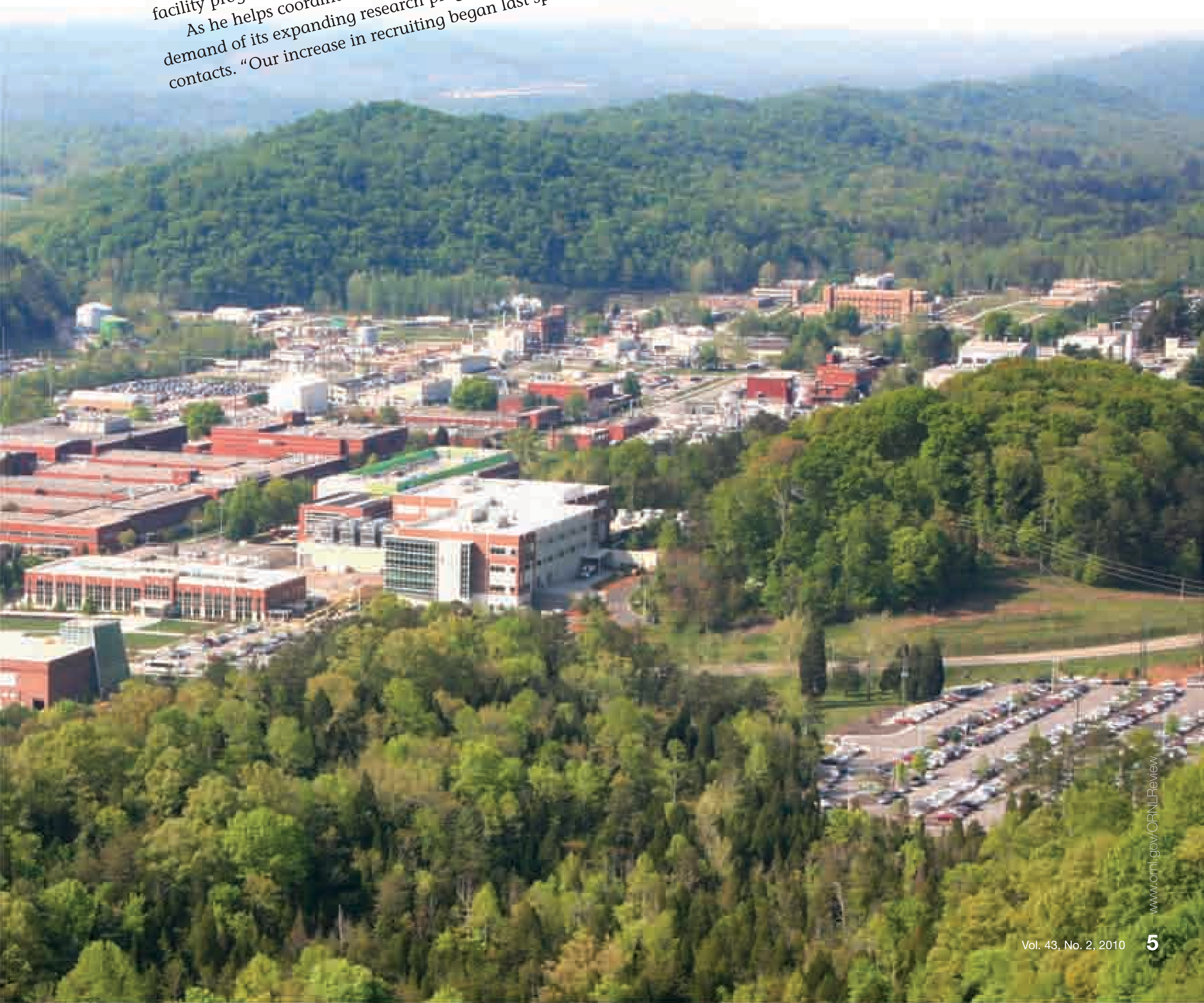
Energy Secretary Steve Chu (center), Rep. Lincoln Davis, Governor Phil Bredesen (left), Director Thom Mason, University of Tennessee President Jan Simek and Battelle President Jeff Wadsworth (right).

DELIVERING THE SCIENCE

With modern facilities, the challenge now is to produce great science.

ORNL is in the midst of the biggest expansion of its scientific staff in more than three decades. Because user facilities play a central role in the laboratory's research program, they are both a part of the reason for the surge in recruiting and beneficiaries of the newly added staff. "DOE would not have located the facilities at the laboratory if we did not have high-quality staff members," says ORNL's Director of Strategic Capabilities, Jim Roberto. At the same time, the user facilities are one of several tools the laboratory uses to create a community of users that can help identify and recruit candidates for staff vacancies. It's not uncommon for new staff members to be former users or to have professional connections to the laboratory through former users. "Our staff has a very extensive network of contacts who can help identify candidates," Roberto says. "This network is built, to some extent, by people who have passed through our user facility programs and have developed research relationships with the laboratory."

As he helps coordinate the laboratory's effort to ramp up recruiting to meet the demand of its expanding research program, Roberto is drawing on many of these contacts. "Our increase in recruiting began last spring when the laboratory learned



ORNL supports research opportunities for students, postdoctoral researchers and scientists from universities and industry.

about growing opportunities in the area of energy research," Roberto says. That's when ORNL received the first of several boosts to its research portfolio, $46 million in funding for the creation of two Energy Frontier Research Centers to further research into energy storage and the basic properties of materials. "We surveyed our research divisions to try to understand what the scientific and technology needs of the laboratory would be through the end of 2010," Roberto explains. "Altogether we identified close to 500 science and technology positions." Over the last year, ORNL has filled about half of these, leaving another 260 to fill in 2010. "Growth in the laboratory's research programs has occurred across the board," he says, "with the biggest increases in the areas of computational science and energy and engineering science."

Roberto notes that major scientific centers, like ORNL's 11 user facilities, play a significant role in attracting quality scientific staff to the laboratory. "Scientists come to ORNL because of the quality of our people, their interest in our portfolio of research programs and the opportunity to work with world-class facilities," Roberto says. One of the many ways in which ORNL cultivates interest in its research programs is by supporting opportunities for students, postdoctoral researchers and scientists from universities, industry and other research institutions to come to the laboratory and participate in both long- and short-term research projects. Many of these visiting researchers conduct their own research at one or more of the laboratory's user facilities; others are involved in a range of research and development activities, from internships to collaborations to fellowships. "All of these programs are important in the creation of a large cadre of people who are familiar with the laboratory, what we do and the opportunities that exist here," says Roberto. "This has been a very effective recruiting tool for us."

Other effective recruiting tools are the research facilities themselves. Roberto is quick to point out that the design, construction and operation of major national research facilities are among the unique mission roles of the Department of Energy's national laboratories. These facilities are located at national laboratories because only laboratory-scale organizations can provide the large multidisciplinary teams needed to design them, oversee their construction and operate them successfully. Roberto contends that the scope of DOE's research facilities is unique in the world. "There is no agency on earth that has as many leading facilities in as many areas as the DOE system," he says. "We have world-class synchrotrons, neutron sources, accelerators, computational facilities, nanoscale science centers and much more."

ORNL is home to many of DOE's leading user facilities and has been fortunate in recent years to have been selected to host several more, such as the Spallation Neutron Source, the Center for Nanophase Materials Sciences and the Oak Ridge Leadership Computing Facility. Roberto observes that the value of these facilities goes well beyond providing world-class tools for ORNL scientists: "These facilities strengthen the research fabric of the nation and promote scientific interactions and partnerships across a broad range of disciplines with leading institutions across the country and around the world." Ⓡ

An Unbeatable Combination

ORNL's neutron sciences program is in the enviable position of having a user program that combines access to the Spallation Neutron Source (SNS), the world's most powerful pulsed neutron source, with entrée to the High Flux Isotope Reactor, the world's most powerful steady-state neutron source. This combination provides users with unusually well-rounded, some would say unmatched, materials characterization capabilities.

Neutron Sciences Director Ian Anderson explains that the instruments at these two facilities give scientists complementary views of the structural and dynamic nuances of material samples.

At the High Flux Isotope Reactor the neutron beams are continuous, so the instruments there are excellent for looking at molecular detail inside relatively stable materials. The SNS, on the other hand, produces neutron beams in very intense pulses—60 times a second. These pulses are perfect for looking at things that are changing quickly. The reactor is the bright lamp, while SNS is the stroboscope.

The advantage of having both of these facilities at ORNL is that a researcher can make both kinds of measurements on a range of instruments at a single institution, rather than having to go to multiple facilities to gather comparable data. Anderson cites the example of ongoing studies of a group of complex molecules called dendrimers, or "starburst" polymers. Conventional wisdom was that these dandelion-shaped molecules changed size in response to changes in the electrical charge or acidity of their environment.

"At the High Flux Reactor, we conducted studies to test the assumption that increased electrical charge or acidity would increase the size of the molecule," Anderson says. "In this case we were looking at the low-resolution structure of the material, the size of the entire molecule, not at individual atoms." The point of determining whether the size of these molecules changed was to determine whether they could be applied to tasks such as delivering drugs to specific places in the body. Because the polymer can be made to look benign to other cells, including cancer cells, it could be engineered to be absorbed by them. Then, once inside the cell, the polymer could deliver a pharmaceutical payload, rather like a Trojan horse.

Measurements made at the reactor indicated that, despite changes in the distribution of the atoms in the molecules, the size of the molecules themselves remains more or less the same. Researchers then took the samples across the ORNL campus to the SNS to determine how the molecules moved under the same conditions and exactly how their distribution changed. All these factors will help determine the suitability of these molecules for a range of applications.

Anderson stresses that a researcher coming to ORNL can choose the instrumentation at each facility that is best adapted to making the necessary measurements and then combine the results to get a comprehensive look at the material being studied.

More than one-half of the users in the neutron sciences program currently conduct research at both the SNS and the High Flux Isotope Reactor during their stay at the laboratory, but for some the attraction does not end there. "Some users are particularly attracted to ORNL by the analytical capabilities of the reactor and the SNS combined with the nanoscale engineering capabilities of the Center for Nanophase Materials Sciences," Anderson explains. "So in one project a researcher can synthesize a material at the nanocenter and make multiple measurements of its structural and dynamic characteristics at both the reactor and the SNS without leaving the site."

In fact, visitors to ORNL have access to an unusually broad range of materials characterization capability. "When you include ORNL's SHaRE microscopy facility, the High Temperature Materials Laboratory's materials measurement characterization capabilities and our world-class computing facilities," Anderson says, "one realizes that ORNL has a combination of capabilities that would be hard to match anywhere in the world."

Artist's rendering of the laboratory's guest house.

A PLACE TO SLEEP

As if a suite of world-class research facilities was not enough, by early 2011 ORNL will have an additional attraction for potential users when the new guest house will have opened its doors to the laboratory's visiting scientists. Located just down the hill from the Spallation Neutron Source (SNS), the facility will be particularly convenient for users at the SNS and the Center for Nanophase Materials Sciences, many of whom often work on experiments that run at all hours of the day and night.

Similar to a small, on-site hotel, the guest house will have 47 units, including a mix of single and double rooms. The rooms will be equipped with amenities that include televisions, microwave ovens and wireless internet access. The facility will include a lounge area, vending area, breakfast area, meeting room, fitness room and guest laundry room. The facility will also be outfitted with a "prep" kitchen, opening up the possibility of serving continental breakfasts or preparing food for special events. The proximity of the guest house to the SNS office building will also provide guests easy access to the SNS cafeteria and fitness center.

Ground was broken for the facility in February, and the building is expected to be ready for occupancy by early spring of 2011.

PULSING INTENSELY

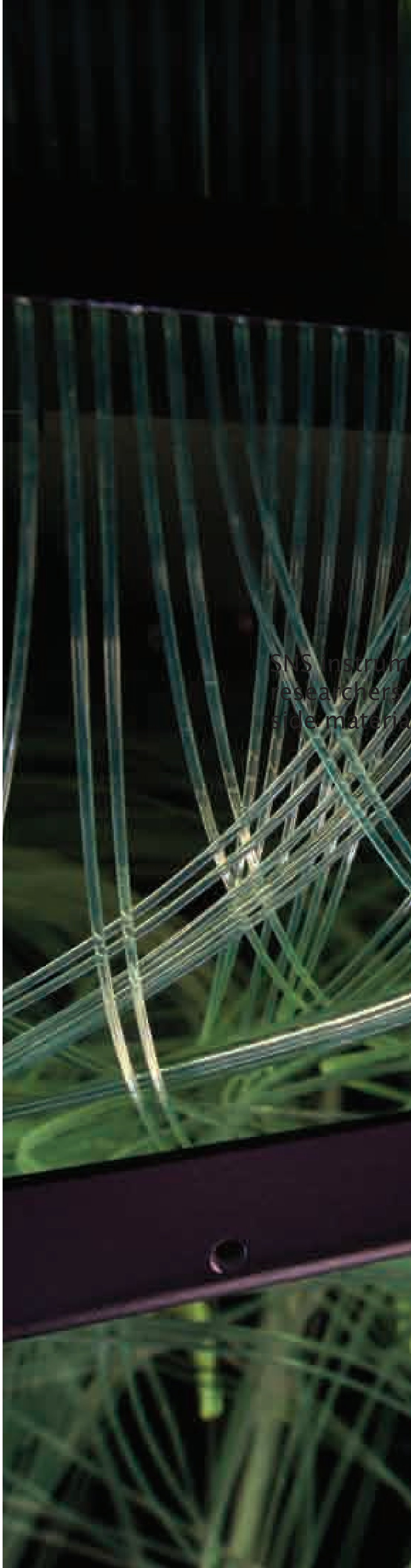
SNS instruments enable researchers to "see" inside materials.

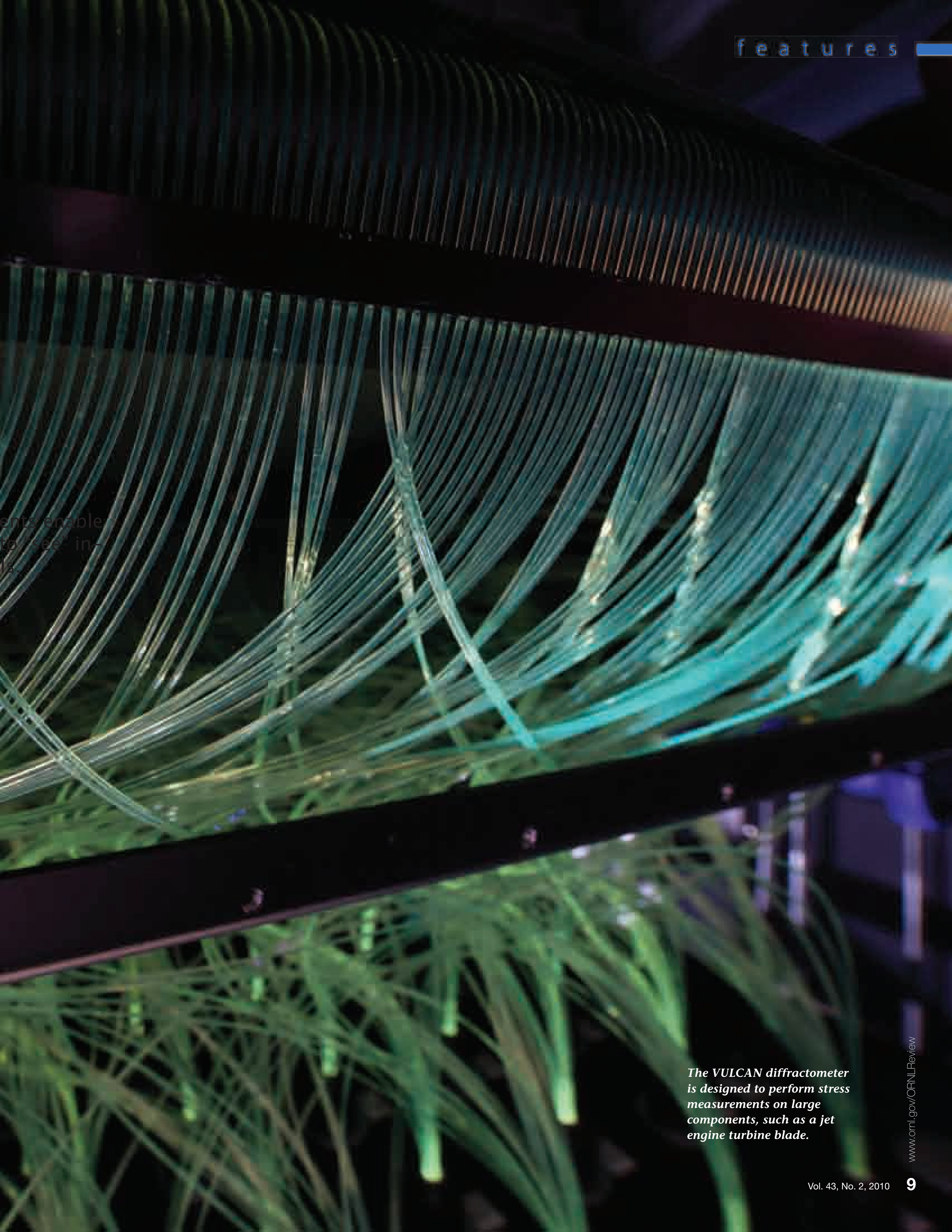
Four years after a keystroke produced the first neutrons, the Spallation Neutron Source (SNS) has moved into a new phase, both as a neutron research facility and as one of the scientific community's foremost user centers for materials research. "We now have the world's most intense pulsed neutron source, a fact that by itself is very attractive to anybody who wants to use neutrons to investigate materials," says Stephen Nagler, chief scientist of ORNL's Neutron Scattering Science Division. Adding to the facility's appeal is the realization that, with every new operating cycle, the SNS is putting more instruments with brand new capabilities online. Twelve instruments, some as large as houses, are currently available in or adjacent to the mammoth target building, with seven more under construction or in the process of coming online.

Users are flocking to the new instruments. Typically, once an SNS instrument becomes available, user requests for research time run about a factor of three greater than the amount of time actually available. Proposals for some of the newer instruments are running six or seven to one. While the perfect balance is elusive, the SNS staff closely monitor the nature and quality of the proposals as well as the ratio of accepted proposals. Just as a healthy ratio serves as an indicator that the instrument is attracting great science, a ratio that becomes too high could deter quality users from submitting proposals.

One of the newest and most popular SNS instruments is the VULCAN diffractometer. The reasons behind VULCAN's popularity—a new machine with unusual capabilities—are similar to those that make the SNS itself so attractive. VULCAN was designed to perform stress measurements on engineering components such as a turbine blade from a jet engine or the frame of a car. VULCAN is capable of "seeing" inside the material and making three-dimensional maps of the distances among atoms in critical sections. The maps enable scientists to determine if the atoms are being squeezed together or pulled apart, signs of stress and strain in the materials.

Studies similar to those conducted at VULCAN have been under way for years at the Residual Stress Facility at ORNL's High Flux Isotope Reactor. The research reactor generates a continuous beam of neutrons of various wavelengths. A larger volume of neutrons hitting the sample often translates into more data. However, to conduct stress and strain measurements, scientists can only use neutrons of one wavelength at a time while filtering out the rest. The extreme intensity of HFIR's neutron beam enables this technique to achieve good results even after filtering most of the neutrons. In contrast, VULCAN produces neutrons in very short bursts. Because the short-wavelength neutrons in the pulse travel faster and arrive sooner than those with longer wavelengths, neutrons of different wavelengths are not mixed together. The result is that all of the neutrons arriving at VULCAN can be used to take measurement samples. A bonus for VULCAN users is simple logistics. Because VULCAN is located in a separate and spacious building, the movement of large samples to the instrument, such as a section of aircraft wing, becomes much easier.





The VULCAN diffractometer is designed to perform stress measurements on large components, such as a jet engine turbine blade.

Nagler also views VULCAN as a good example of ORNL's efforts to broaden the neutron science user base. He points out that the application of neutrons to engineering studies was something that followed long after they were first used in areas such as solid state physics. Interest among engineers began with users examining topics like residual stress in materials. That initial interest has expanded to include the use of pulsed neutrons to investigate energy materials such as photovoltaics, fuel cell membranes and related devices. Nagler expects a continued increase in the number of users attracted to neutron science at the SNS for applied materials research. He also predicts a similar growth in other fields like materials chemistry. "There has been occasional work of this type in the past," Nagler adds, "but the SNS is attracting a much broader group of researchers to the field."

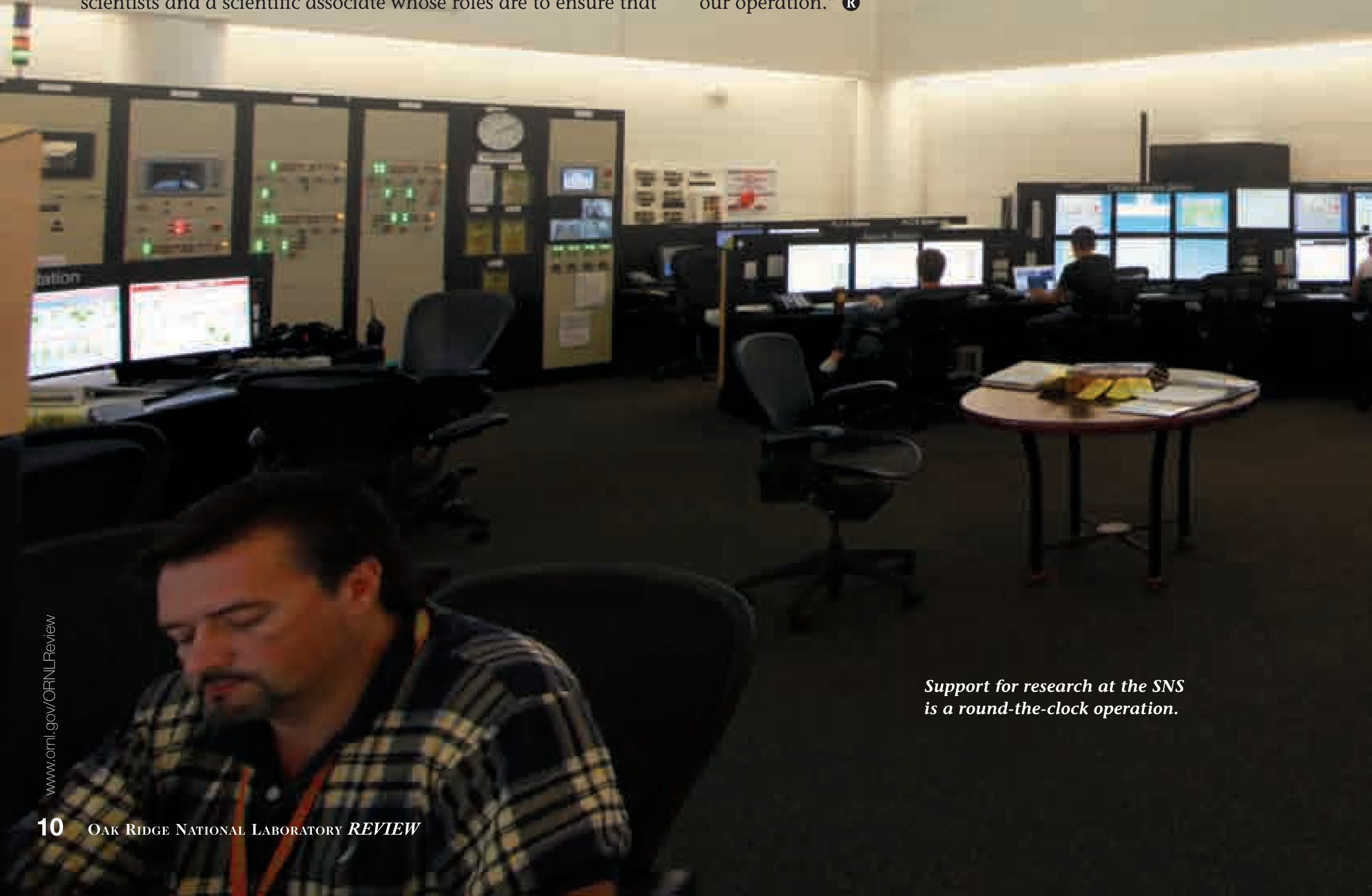
As awareness of the SNS and its capabilities grows, potential users are gradually realizing that the additional data obtained at the SNS positions them to perform experiments that would be impossible elsewhere. At the SNS, users have the twin advantages of working with instruments designed on the basis of knowledge gained from decades of experience at neutron facilities around the world, powered by a peak neutron flux ten times that of similar facilities in Europe and Asia. The difference is profound.

Users come first

To maximize access to these capabilities, 75 percent of the beam time on SNS instruments is dedicated to the general user program. Each instrument typically has one or two instrument scientists and a scientific associate whose roles are to ensure that instruments are operational when users arrive to conduct their experiments. "The support is not limited to instrument scientists and scientific associates," Nagler explains. "We have a group that specializes in maintaining samples in specialized environments, such as low-temperature, high-temperature or some special atmosphere or condition. Those who work for this group support each experiment as well." Because the SNS staff members are well known for their subject matter expertise, users frequently collaborate with them to take advantage of their ability to interpret data and set up difficult measurements. "This support is not a requirement," Nagler notes. "Some users prefer to do their own thing and get technical assistance only when they need it. We provide the support either way."

Research at the SNS is a round-the-clock operation. When scientists are awarded beam time, they are expected to work until their experiment is complete. The policy requires continuous support, with a "hall coordinator" in the experiment hall 24 hours a day, seven days a week. If users are running an experiment and encounter a problem, the hall coordinator will either fix the problem or identify those who can.

Because the SNS is the first U.S. neutron facility built in decades, ORNL has made a priority of making the user experience successful. Nagler makes clear that, despite the facility's initial success, the SNS staff is not resting on its laurels. "Every time a user runs an experiment, he or she is asked to provide feedback on how things went and to critique what could have been better," he says. "The feedback is taken seriously. Users are a critical part of our mission, and we are constantly looking for ways to improve our operation." Ⓡ



Support for research at the SNS is a round-the-clock operation.

Investigating layered thin films

Svetlana Sukhishvili is a professor of chemistry and co-director of the Nanotechnology Graduate Program at Stevens Institute of Technology in Hoboken, New Jersey. As part of the Spallation Neutron Source's (SNS) user program, she and her students are using the facility's Liquids Reflectometer to study layered polymer films. These thin films are composed of polymer layers of varying composition, built up one layer at a time. "These layered films currently have many potential applications in controlled delivery, as well as in optics as antifog coatings and antireflective coatings," she says. "However, very little is known about the internal structure of such films." The Liquids Reflectometer provides a way for scientists to look within and between the layers of film and determine how they are structured and how those structural features are related to the film's properties. "We asked several questions," Sukhishvili says. "When we are depositing polymer layers on surfaces to make films, will these films remain layered when used in wet environments? Also, if the internal structure changes, under what conditions does it change and how does this affect the internal structure of the film?"

One of the technology's applications is controlled delivery, or "time-release" delivery of functional small molecules. This behavior could be utilized in a drug delivery system or as a coating on the surface of a biomedical device that would release different compounds at predetermined times. The polymer layers can trap small molecules and then release them on demand or in response to changes in environmental conditions, such as temperature or acidity. "For these films to function properly, it is important that the layers remain well structured," Sukhishvili explains. "This depends on the dynamics of the polymer molecules at the layer boundaries, which are not not well understood."

Sukhishvili's group created their films by depositing layers of material containing deuterium, an element that is easily "seen" by neutrons, with hydrogen-containing layers in between. The purpose of having alternating layers containing deuterium and hydrogen is to provide contrast between the layers at their interfaces. "We wanted to look at how the structure would spread when we changed the environmental conditions. We found interesting trends between the strength of intermolecular interactions and intertwining of polymer layers and the structure of the films." Sukhishvili points out that using alternating layers of deuterated and hydrogenated materials to enhance contrast is a unique technique and is well suited to the capabilities of the SNS. "We are one of the few groups in the country that decided to take advantage of the SNS to look at this fundamentally important, yet practically relevant, question to shed some light on the structure-property relationships of such films," she says.

Sukhishvili views the SNS as a new kind of user facility that offers broad opportunities for networking and collaboration. "The SNS is a growing and forward-thinking user facility," she says. "I also think the potential for collaboration with ORNL's Center for Nanophase Materials Sciences and the combination of these capabilities with the ability to do new and exciting neutron reflectivity experiments provide much broader options. The result, she believes, will be an attraction to users for years to come.

Optical fibers of a VULCAN detector module


X05
X04
X06

THE NEXT SMALL THING

An unconventional approach attracts users to ORNL's nanocenter

Oak Ridge National Laboratory's Center for Nanophase Materials Sciences (CNMS) is one of five Department of Energy nanocenters with a unique mission. While most user facilities focus on measuring and characterizing a variety of materials, from the exotic to the mundane, the nanocenters are designed to develop and study materials that have never existed. "All five of the nanocenters concentrate on synthesizing and understanding new materials as opposed to analyzing samples that people bring in," says CNMS User Program Manager Tony Haynes. He notes that because the research at ORNL's nanocenter is geared toward new materials, users' projects

The Nanocenter (left) is adjacent to the Spallation Neutron Source and just a few yards away from the newly constructed Joint Institute for Neutron Sciences.

tend to be somewhat less conventional and less predictable than those at other facilities. "We do not have the material in hand that we want to study, or even the recipe for making it," Haynes explains. "We usually try to make a material that has a particular set of properties, learn what we can from the process, and then repeat the process again and again to improve the result and to understand the new material."

One effect of this ground-up approach to research projects is that user requests for time at the nanocenter are longer than most. Nanocenter projects average 25 to 30 days, compared to three to five days at one of ORNL's neutron scattering facilities. Part of what makes the nanocenter attractive for these longer-term projects is access in a single location to a diverse collection of synthesis and characterization activities. Users who could perform portions of their research at their home institutions often find it more practical to complete the entire experimental process at ORNL. The nanocenter even provides theory capabilities that users can tap to guide or support experimental projects.

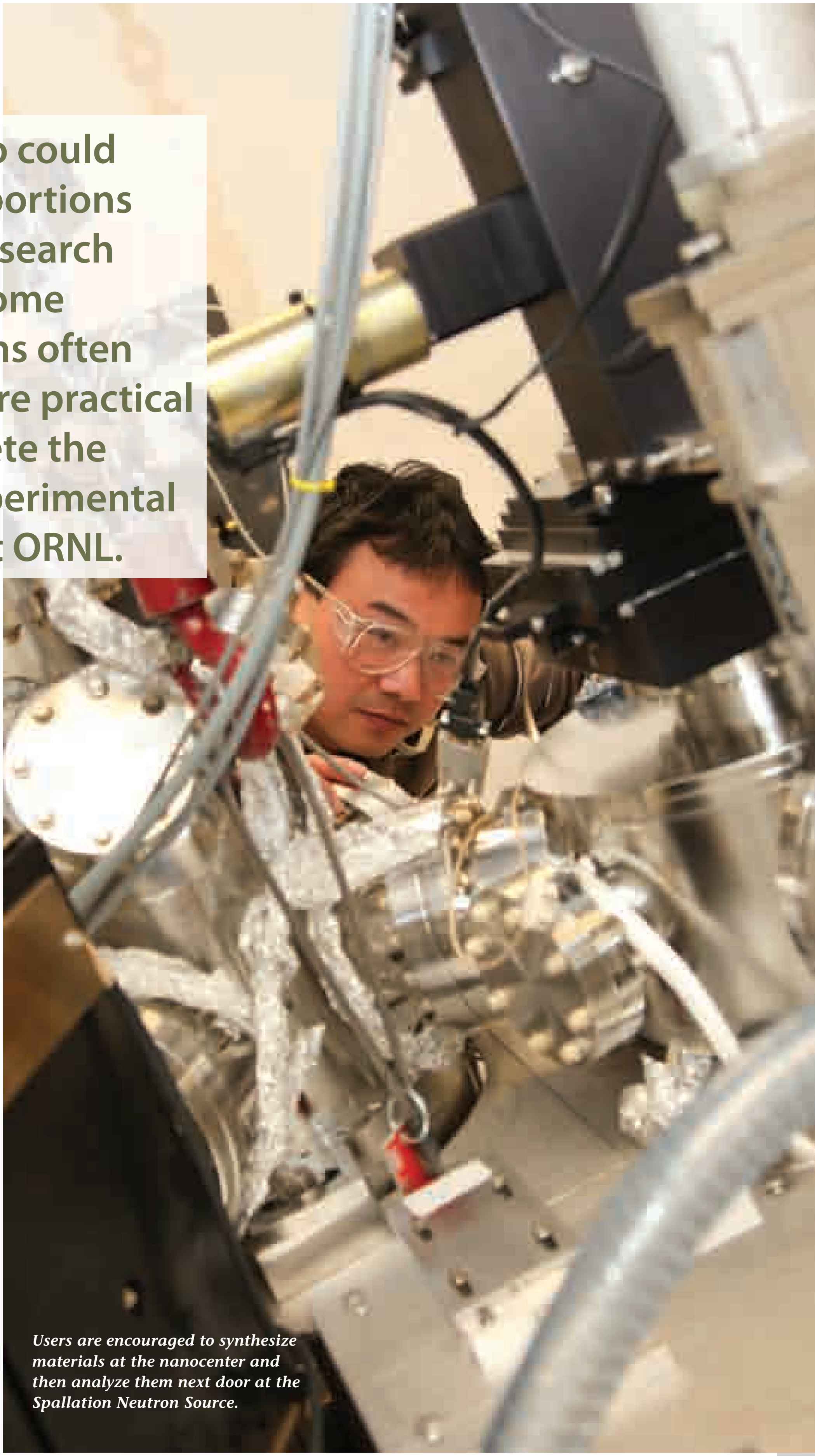
While the nanocenter's state-of-the-art equipment is an attraction for users, their research efforts often get a bigger boost from the capabilities of CNMS staff scientists. Haynes says users generally come to the center with their own notions about how to create the properties of proposed new materials or modify existing materials. "They might have an idea of the atomic structure or chemical composition that could make a material suitable for an application. They come Oak Ridge either to make the material or to have our staff perform theoretical calculations to validate their ideas. As part of the process, we help them test the material for the properties and functionality they originally envisioned."

To provide this support, CNMS scientists must be experts in both making and testing new materials to help users create or modify materials in such a way as to generate specific properties or physical characteristics. Haynes describes the nanocenter as being "in the business of embedding functions in new materials—thermal conductivity, for example, or mechanical stiffness." Once the materials are created, the nanocenter has an unusually large assortment of analytical tools and techniques to aid users in probing the structural, chemical, physical and other properties of their creations.

Neutrons for neighbors

Apart from distinctive capabilities, ORNL's nanocenter is also known for its distinctive location, adjacent to the Spallation Neutron Source (SNS), the world's most powerful pulsed neutron research facility. While convenient, the proximity does not by itself give CNMS researchers an unfair advantage in the competition for research time at the SNS. "There is, as one would hope, substantial research collaboration between the nanocenter and the SNS," Haynes says, "but there is no special 'deal' between the two facilities." CNMS scientists must go through the same rigorous proposal procedure as other researchers to conduct an experiment at the SNS. Haynes acknowledges that proximity to the SNS does make it easier for CNMS scientists to collaborate with their SNS colleagues who already have been awarded allocations of time on various instruments. "We often make materials that neutron scattering experiments can help us understand," he says, "so we sometimes collaborate with SNS scientists who are interested in our research, the kind of collaboration that any researcher in the world can propose."

Funded by the Department of Energy's Basic Energy Sciences program, both the nanocenter and the SNS strive to simplify the procedures for users to propose and conduct experiments that involve synthesizing materials at the nanocenter and then analyzing them with the massive neutron instruments next door. Haynes is convinced the "cross-pollination" between disciplines produces innovative science. "The growth of new ideas among scientists from different research communities is the long-term benefit of these facilities being located together."



Users are encouraged to synthesize materials at the nanocenter and then analyze them next door at the Spallation Neutron Source.

Producing a breakthrough

As a classic user facility, the Oak Ridge nanocenter provides visiting scientists with access to equipment that is unavailable in their own institutions. An added benefit is the opportunity for users to conduct research that also transcends the limitations of their staff. While scientists sometimes can perform 90 percent of their research without coming to CNMS, Haynes suggests the combination of equipment and staff capabilities is what users often need to produce a breakthrough. Ⓡ

Venkatraman Gopalan

One goal of user facilities such as the Center for Nanophase Materials Sciences (CNMS) is to enable researchers to answer basic questions about why materials behave as they do. One such project involves a ferroelectric material being studied by Venkatraman Gopalan, a professor of materials science and engineering and associate director for the Center for Optical Technologies at Penn State University, and his student, Vasudeva Rao Aravind. Much of the research conducted at the nanocenter involves new kinds of material; however this material has been valued for its unique properties for decades, yet retains a number of fundamental mysteries.

Gopalan and Aravind used the scanning probe microscopy facilities at CNMS to study a specific feature, called a domain wall, of a class of crystalline materials called "ferroelectrics." Ferroelectric materials are notable primarily because they are naturally polarized. One end of the material can be positively charged and the other negatively charged, giving them a net polarization direction. The polarization "up" and polarization "down" domain states of the material are separated by a boundary called a domain wall. When an electrical current is applied to these materials, the polarization of the ends can be "flipped," or reversed. This behavior makes the materials useful in applications, such as small piezoelectric motors, nonvolatile memory and other electronic and optical devices.

"One of the interesting things about ferroelectrics," Gopalan says, "is that despite using them for 60 years we are still learning new things." The research conducted by Gopalan and Aravind focused on determining the structure of the domain wall. Gopalan points out that, "We can determine some features about the wall from textbooks, but there are still mysteries that remain unresolved. That's what this project was about."

Working at Penn State, Gopalan and Aravind came to believe that the domain wall has properties that are significantly different from those of the rest of the ferroelectric material. "In a ferroelectric material, the wall is very 'sharp,' or narrow, one or two crystal cells wide," Gopalan explains. "It is so narrow that researchers generally don't think about the properties of the wall itself and are more concerned with the bulk properties of the whole material." However, Gopalan and Aravind surmised that the nanoscale properties of the wall might be very important to understanding the material as a whole.

The two researchers did some preliminary experiments to test their theory that one of the distinctive properties of the wall is an electrical "softness," meaning that only a small voltage is required to flip the polarization of the material if the voltage is applied close to the wall. A much larger voltage is needed to achieve the same result if applied farther away. "Our results suggested this could be possible, but we didn't have the kind of sophisticated scanning probe microscope that would be needed to achieve definitive results." That's where the CNMS scanning probe microscopy facilities came in. "At the nanocenter," Gopalan says, "Sergei Kalinin's group has not only a very sophisticated scanning probe microscope, but they have also developed unique software that automates the process of scanning and mapping the crystal."

Aravind made several multiweek trips to the Oak Ridge to study the structure of the wall. "After the first trip, we had a sense of where this experiment would go," Gopalan recalls. "By the second trip, he was seeing amazing results. He mapped beautifully how the wall has a life of its own. We found that the area near the wall is 10 times electrically softer than the areas further away. This is the first direct measurement of such a thing. None of the textbooks describe anything like this."

Members of Sergei Kalinin's group receive high praise from users for their experimental techniques and for their ability to help users maximize their research.

Gopalan adds that while the structure and electrical nature of the ferroelectric domain wall had recently been theoretically predicted, no direct measurements of the phenomenon existed until this experiment. "Our research group has analyzed the results using several different models to try to explain them because this behavior is so basic to understanding ferroelectric materials," he says. "Now we have a model that enables us to understand why the domain wall behaves as it does. We have theories and predictions that match our experimental results."

Gopalan emphasizes that the nanocenter played a valuable role in unraveling a little more of the mystery of the ferroelectric domain wall. "I don't know of a better facility, particularly in the area of piezoelectric force microscopy." He adds, "Sergei Kalinin's group is doing pioneering work in this field. They have not just developed their techniques, but they have taken their approach to the research to a new level. These guys are some of the best in the world in their field. We want to collaborate with them, not just to get access to their facilities and collect high-quality data but also for their intellectual inputs in interpreting and understanding the data. That's where their real value comes in."

MAGIC SECRETS

Researchers use "magic nuclei" to unlock the secrets of heavy elements.

The Holifield Radioactive Ion Beam Facility has the ability to create and analyze isotopes that exist for just a few seconds.

Inner space and outer space: Representing the bookends of atomic discovery, they are the two big attractions for the hundreds of visiting scientists who each year conduct research at ORNL's Holifield Radioactive Ion Beam Facility. Holifield's ability to create and analyze isotopes that exist for only seconds gives researchers a unique glimpse into the inner workings of atomic nuclei, as well as how they interact with each other and with high-energy particles. Understanding these processes provides astrophysicists with insights they will need to continue to unravel the mystery of how the same processes could have created of all of the heavy elements in the universe, both in the hearts of stars and through hyperviolent stellar events such as supernovae.

Holifield's users are primarily scientists from national and international universities. "This year we have about 200 users either on-site or working on studies waiting to be run," says Carl Gross, who manages the facility's experimental systems. "Additionally, we have more than 500 'potential users' who stay up-to-date with Holifield's research and capabilities. Last year's workshop on Holifield's wide-ranging capabilities attracted more than 150 participants from 44 institutions and 10 countries. Scientific director Witold Nazarewicz believes interest is increasing because of Holifield's unique capability to produce and study beams of the short-lived isotopes created by fission reactions.

Holifield holds the distinction as the only American facility that generates radioactive ion beams using the isotope separator online technique. The technique accelerates protons that strike a uranium target, which then fissions into a spray of different isotopes. Researchers focus and accelerate this assortment of short-lived elements into a beam for analysis. The isotopes produced by this process include those found in stars, as well as those created as fuel is consumed in nuclear reactors. "Many of these isotopes have only been detected and never studied in any detail," Gross says. "We are able to analyze them with a range of sophisticated measurement tools to see how they interact with one another."

"Magic" nuclei

One scientist benefiting from Holifield's singular capabilities is Kate Jones, an assistant professor at the University of Tennessee. Her studies focus on what she describes as "a junction point between three areas of physics research: nuclear structure, nuclear reactions and nuclear astrophysics." The object of many of Jones's subatomic inquiries is the behavior of the somewhat enigmatic isotope tin-132. Although its fleeting, 40-second half-life makes working with tin-132 difficult, the isotope is significantly more bound than its atomic neighbors and has a number of characteristics that endear the isotope to nuclear physicists.

Researchers are exploring how neutrons and protons (known collectively as nucleons) in the nucleus influence its shape and behavior. Nuclei carry a number of layers, or "shells," of either protons or neutrons. Each shell in turn can carry a limited number of nucleons. Once a shell is full, or "closed," adding or removing a nucleon becomes more difficult, resulting in nuclei with full shells that tend to be more stable than those with incomplete or "open" shells. Tin-132 is of special interest to nuclear structure physicists because it has closed shells of both protons and neutrons. Because tin-132 has many more neutrons than protons, the isotope also appeals to researchers seeking to understand why such nuclei tend to be unstable.

With its closed shells, neutron-heavy tin-132 provides a platform upon which to study the effect of adding a single nucleon to the nucleus outside the doubly closed shells. "At Holifield," Jones says, "unstable nuclei like tin-132 nuclei can be accelerated to an energy that enables us to add a neutron to the nucleus, creating tin-133. The neutron is added to tin-132 by causing it to collide and react with a deuteron (a deuterium nucleus, consisting of a neutron and a proton). By measuring the energy and angle of the proton emerging from the reaction, invoking conservation of energy and momentum, we can determine exactly how the neutron is incorporated into the new tin-133 nucleus." Jones adds that Holifield is the only place in the world with the capability to study these isotopes in this manner.

"At Oak Ridge we are unique both in terms of the isotopes we produce and the intensity of our beam."

Hearts of stars

One of the most important quests in nuclear science is the effort to understand how heavy elements are created. From hydrogen to iron, elements can be created by nuclear fusion in the hearts of stars. However, creating heavier elements requires energy consumption—rather than energy production, as is the case of lighter nuclei—suggesting there is another path for the creation of the elements from iron to uranium. Scientists theorize this creation process for heavier elements occurs in two basic contexts: very quickly (on the order of seconds) in supernovae and other violently energetic cosmic events, and very slowly (typically thousands of years) in the hearts of light- to intermediate-mass stars late in their lives.

Isotopes like tin-132 that have nuclei with closed shells of both protons and neutrons and an overabundance of neutrons are of interest to physicists not only because of what they reveal about the structure of nuclei, but also because they are thought to influence key astrophysical phenomena, such as the formation of heavier elements. The structure and behavior of tin-132 provide scientists insight into the nuclear reactions that occur within astrophysical phenomena such as supernovae. Some theorize that during these explosions neutrons are captured by nuclei, leading to the formation of the heavier elements.

Tin-132 represents an extremely important benchmark, both for understanding nuclear structure and for calculating the properties of the plethora of nuclei involved in producing heavy nuclei in explosive cosmic events such as supernovae. Most such nuclei are so exotic and so short lived that they are not available for experimental study. Their properties and reactions, therefore, must be modeled.

Jones explains that "rather than fusing nuclei to create heavier elements, these elements can be created by fusing neutrons into the nuclei of atoms." This process does not create a heavier element, producing instead a heavier isotope of the same element. When enough neutrons have been added to the nucleus to make the element unstable, the nucleus decays. This process converts one of the added neutrons into a proton, thus creating a different element.

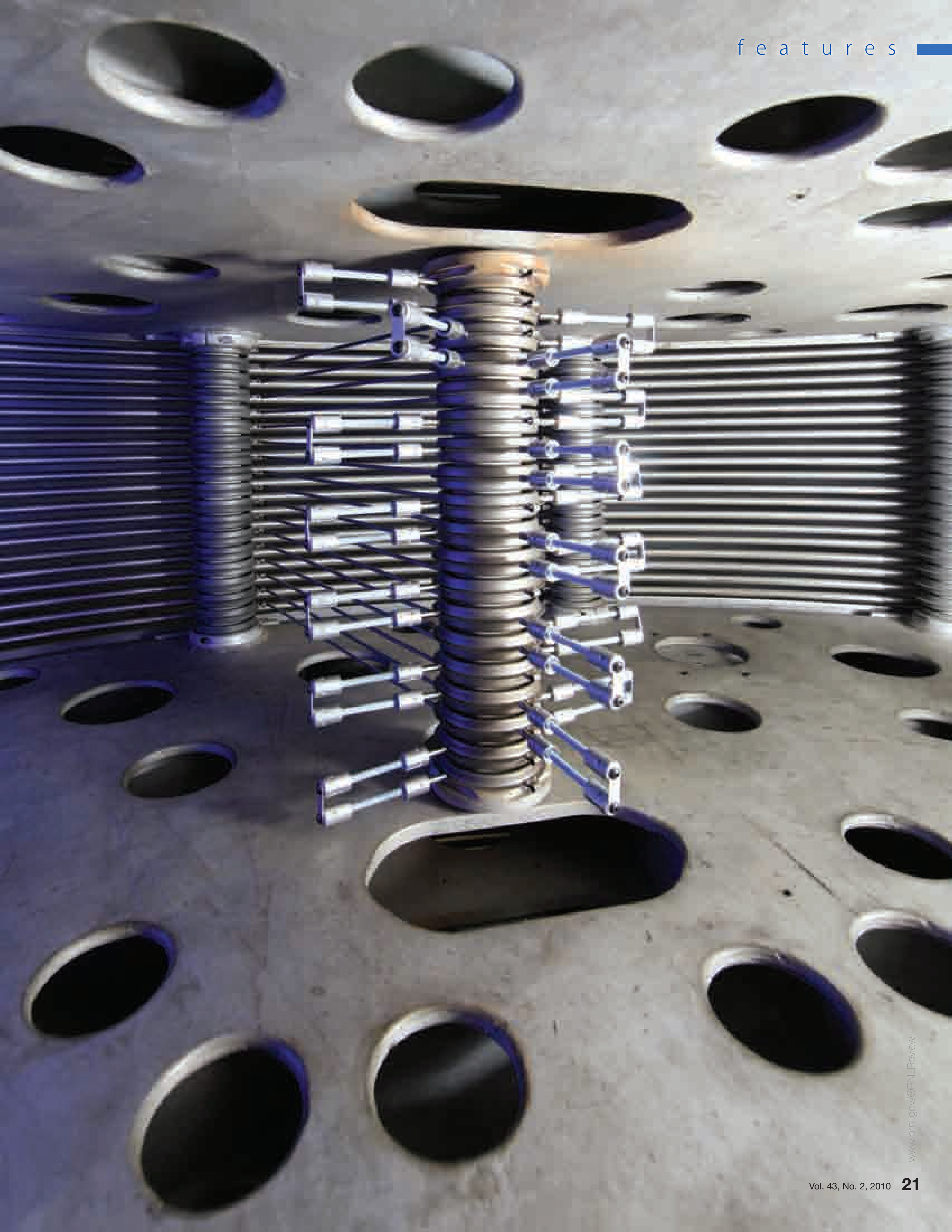
Computer models that incorporate the rate at which neutrons are captured by isotopes neighboring tin-131 in supernovae have indicated these isotopes may play a critical role in determining the quantity of heavier elements produced by supernovae. Jones and her colleagues are experimenting with tin-132 and nearby isotopes to try to identify the details of this process. If the team is successful, their findings can be used in models to determine how other factors, like a star's size or magnetic fields, contribute to the synthesis of new elements.

The only game in town

While there are many approaches to studying the mechanics of the atomic nucleus, Jones notes that Holifield has the distinction of being America's only facility that produces beams from the fission of uranium. "That makes very neutron-rich isotopes," she says. "If users require the range of neutron-rich nuclei we work with, they must come to Oak Ridge."

Nazarewicz also emphasizes Holifield's one-of-a-kind capabilities. "Although there are other radioactive ion beam facilities in the U.S. performing similar work, they specialize in other isotopes because they use a different process to produce their beams. At Oak Ridge we are unique both in terms of the isotopes we produce and the intensity of our beam." Nazarewicz points out that Holifield users specialize in creating and analyzing isotopes to help answer key questions about nuclear structure, as well as the origin of the elements from iron to uranium. "These are actually very hot areas of science," he says, "particularly with regard to nuclear theory and astrophysics. For users who are interested in these areas, we are the only game in town." R

The charging chains of the Holifield facility are used to produce the 25 million volt potential at the terminal of the Holifield accelerator.



A HELPING HAND

Users find a collaborative environment in which to probe materials.

For more than three decades, ORNL's Shared Research Equipment (SHaRE) User Facility has provided researchers from universities, industry and other national laboratories with two unique commodities: access to an unmatched array of state-of-the-art electron microscopes and collaboration with a highly skilled staff of scientists. These combined resources enable SHaRE's users to investigate and solve previously intractable problems in the fields of materials science, microscopy, physics and chemistry.

As a result of the facility's singular research capabilities, competition for the opportunity to conduct work at SHaRE is intense. Potential users must submit project proposals for review by the facility's proposal review committee, which consists of the nation's top materials scientists and microscopists. SHaRE's director, Karren More, explains that the facility is not only selective in terms of the research proposals accepted, but also looks for research that will maximize the facility's capabilities. "We ask users to justify why they need these specific instruments to do their research," More says. "They're very specialized instruments, so want to ensure they are reserved for only the best science."

In the case of SHaRE, "the best science" runs the gamut of basic materials science issues, as users investigate the structure, composition and chemistry of a wide range of materials. "We have proposals to do just about everything," More says, "but our focus is on solving materials problems that require high-resolution analytical electron microscopy."

Because SHaRE has a variety of specialized electron microscopes, users can examine features of materials that are measured in millimeters down to millionths of a millimeter. Researchers can also examine the same material with different techniques. More says that scientists can probe a material's topography, morphology, grain boundary structure, atomic structure and composition, depending on the type of study the user is conducting. "All of their activities are ultimately related to the physical and chemical structure of the materials with which they are working," she says. "By studying the properties of the materials, they are conducting very fundamental research to understand the mechanisms of how materials behave."

An interactive research environment

Like most of ORNL's user facilities, SHaRE maintains an in-house research mission, as well a user program. When not supporting users, staff members conduct independent research focused on achieving an advanced understanding of how materials are structured and atomic-scale microanalysis techniques. As a result of this arrangement, SHaRE users have

Users at SHaRE investigate the structure, composition and chemistry of a wide range of materials.

the benefit of collaborating with scientists who continuously work at the leading edge of materials science and electron microscopy research.

More notes that while most users have a clear sense of what they wish to accomplish with their research projects, they often require staff support from SHaRE to help them achieve their goals. "This is a complicated field," she adds. "We do not expect users to conduct their research in isolation during their visits to the lab. Rather, we attempt to provide a very interactive research environment by assigning experienced staff members who work directly with users and help them conduct their experiments. When users collaborate and interact with our staff, the result is a higher quality of research."

Collaboration and interaction

Kevin Field, a SHaRE user and a graduate student at the University of Wisconsin, echoes More's assessment of the importance of the facility's uniquely skilled staff. "When we come to SHaRE, we conduct all of our work with a staff scientist, so we have access to expertise that might not be available otherwise. I have been collaborating with Jim Bentley, a SHaRE scientist who has been doing this kind of work for decades. I have gained tremendous knowledge simply by working with someone who has been in the field for so many years."

Field's research at SHaRE involves analyzing irradiated steel alloys to understand how these materials would respond to radiation if they are eventually used in next-generation nuclear reactors. Part of his research involves using several different SHaRE instruments to examine irradiated steel samples, characterizing the extent of the phenomenon known as "radiation-induced segregation." The condition occurs when atoms have been knocked out of place by energetic particles in such a way that the uniform crystal structure of the steel is replaced by an uneven distribution of certain elements. This reaction can cause the steel to weaken and eventually crack. Stressing that reliability is a critical concern for steel used in reactor vessels, Field explains that he and his colleagues are trying to determine whether this phenomenon also occurs in a variety of steel alloys. "If it does," he says, "we want to understand the factors that cause such conditions to occur."

Kelly Perry is a SHaRE staff scientist, but until a few months ago she was a SHaRE user and a graduate student at Rensselaer Polytechnic Institute in Troy, New York, studying the structure of polybenzimidazole (PBI), a polymer with critical applications in the development of membranes for hydrogen fuel cells. These fuel cells could be used for combined heat and power units in homes, as well as in methanol-fueled backpack power sources for soldiers in the field. Understanding more about the structure of PBI is a goal along the way to developing more efficient, longer-lasting fuel cells.

As a graduate student, Perry's research involved working with SHaRE staff to determine if relationships existed between the structure and physical properties of PBI membranes that had not previously been investigated. During the course of the study, Perry and her SHaRE colleagues found that, because PBI is 90 percent liquid, the membranes are difficult to study with electron microscopy. They also discovered that the material is easily dehydrated and damaged by the electron beams of the facility's microscopes. Perry and her SHaRE colleagues addressed the problem using a cryogenic transfer system that enables researchers to freeze PBI samples using liquid nitrogen and keep them frozen throughout their analysis. The process protects the samples from becoming dehydrated or degraded by the microscope's electron beam. However, Perry points out that analyzing a frozen sample presents its own set of challenges, both in terms of sample preparation and in distinguishing between characteristics of the sample and anomalies that might have been induced by the freezing process. "It takes time, patience and practice to understand many of these specialized techniques," Perry says. "SHaRE has some of the country's best microscopes and most advanced equipment for sample preparation, both of which are required to perform high-quality microscopy."

Something new every day

More stresses that the true value of the SHaRE user facility is its ability to add depth and breadth to the research experiences of users like Field and Perry. "Our specialty is the analysis of the composition of materials. There isn't a similar collection of instruments anywhere in the country for doing this kind of research." More adds, "It's not that other facilities don't have any comparable instruments, but our success comes from combining the array of instruments we have for doing the full range of materials characterization with the expertise of our staff members, who are leaders in the field."

One benefit of these resources is the fact what while many researchers come to SHaRE to examine a material with a specific technique in mind, the advice of SHaRE staff members often leads them to use several other techniques that provide additional insight into their project. Perry says the SHaRE program is about developing new techniques and new ways to look at materials and understand them. Field adds, "My time at SHaRE has probably been the best research experience I could have ever had. I learn something new every day." Ⓡ

Tom Ballard

When Tom Ballard came to ORNL, he already had 35 years of experience promoting partnerships at the University of Tennessee. He got the opportunity to put that **experience to work at the laboratory almost immediately as a string of world-class user facilities came online in quick succession and demand for access spiked. Driven largely by the expanded capabilities of the National Center for Computational Sciences, the Spallation Neutron Source and the Center for Nanophase Materials Sciences, the number organizations having user agreements with the laboratory has increased five-fold in the last four years.**

In addition to managing user agreements, Ballard's Partnerships organization is responsible for the laboratory's intellectual property; licensing agreements; sponsored research; and building partnerships with businesses, industries, entrepreneurs, economic development organizations and colleges and universities.

We asked Ballard about his organization's role in supporting and promoting user programs at the laboratory across the region and around the world.

You have worked at a research university and a national laboratory. How would you contrast ORNL's research collaboration program with that of the university community?

If I had to pick one word to describe ORNL's research collaboration program, it would be "intense." The user program here is more intense than I saw in 35 years in higher education, but that is because DOE has such a strong commitment to user programs. ORNL has a number of industry partners that we have cultivated over the years, and in the last five years the laboratory's collaboration with commercial entities in bioenergy, nuclear technology and other areas has become even more intense.

What do you think users look for at a facility like ORNL?

They come to ORNL because we have unique expertise in addressing some of their most critical research and development problems. If they could find this sort of expertise elsewhere, we wouldn't be involved. Our users are looking for a customer-friendly, seamless process, so they can get in, get their work done and get out. That sort of experience is what we recently focused on with our User Facility Program Process Improvement Team. We spent a year examining every area of the laboratory that touched on the success of our users, and we looked for ways to ensure that the quality of our User Facilities Program is as high as that of our user facilities themselves. As a result of this effort, we made a number of improvements to ensure that our users can get into the laboratory quickly, get the resources they need and get their work done successfully.

How do you view the role of user facilities within the mission of a world class lab?

I think user facilities are an easier way for universities and commercial entities to test drive a national laboratory before getting into a more substantive and longer-term collaboration. They can see what our capabilities are; they can see what our tools are; they can interact with our people, and they can see how we do business. Frequently, users who are introduced to the laboratory through a user program move on to other forms of collaboration, like our Work for Others program, our Cooperative Research and Development Agreement process or even executing a licensing agreement. I think user facilities play a very important role in helping us to build a larger and more robust set of collaborators. This helps the laboratory stay at the forefront of research and development in the areas in which we have nationally-designated user facilities.

What is the biggest challenge associated with our user program?

Over the last few years, the biggest challenge has been managing the growth in the number of users. The exponential growth has come in three areas – our computing programs because of the expanded capabilities of the National Center for Computational Sciences, home of the world's fastest supercomputer; the Center for Nanophase Materials Sciences; and the Spallation Neutron Source, the world's most powerful pulsed neutron source.

More and more, users want to engage these capabilities, so we have had rapid growth in demand for access to these facilities. For example, we processed 35 new user agreements in 2005, and in 2009 we processed 176. That's a five-fold increase.

What opportunities do you see for future collaboration with the region's economic partners?

I have lived in this area my entire life, and I have worked on collaborations between major institutions in this region for 41 years. However, I have never seen a higher level of realization on the part of the economic development community of how important Oak Ridge National Laboratory is to the economic future of the region. Not only have they recognized this fact, but they are now pursuing economic development strategies that focus on collaboration with ORNL. That means the future for collaboration is bright.

Additionally, as we look at the regional economy, we have to consider the spotlight that Tennessee Governor Bredesen has shone on green energy and on the collaborative efforts between ORNL and the University of Tennessee in the areas of solar technology and bioenergy. He has also highlighted opportunities for research at the laboratory in other green energy areas, including battery storage. In the last few months, ORNL has also been the beneficiary of Department of Energy awards of $55 million in additional research funding: $20 million for enhancements to the Buildings Technology Center and $35 million to build a carbon fiber pilot production line.

All of these developments tell the academic, business and research communities that significant opportunities exist for them to take advantage of our user facilities and our research programs to address their research needs, as well as bringing benefits both to the local economy and to that of the broader region.

I think there are many significant collaboration opportunities on the horizon for ORNL. The challenge for the Partnerships group at the laboratory is to get up every day and focus on helping our researchers to be more successful through stronger external connections and to help the local and regional communities capitalize, in appropriate ways, on the unprecedented growth of research and development activities at the laboratory. Ⓡ

ORNL Z-contrast microscope first to resolve, identify individual light atoms

Using the latest in aberration-corrected electron microscopy, Oak Ridge National Laboratory researchers and their colleagues have obtained the first images that distinguish individual light atoms such as boron, carbon, nitrogen and oxygen.

The ORNL images were obtained with a Z-contrast scanning transmission electron microscope (STEM). Individual atoms of carbon, boron, nitrogen and oxygen—all of which have low atomic numbers—were resolved on a single-layer boron nitride sample.

"This research marks the first instance in which every atom in a significant part of a nonperiodic material has been imaged and chemically identified," says Materials Science and Technology Division researcher Stephen Pennycook. "It represents the most recent accomplishment of the combined technologies of Z-contrast STEM and aberration correction."

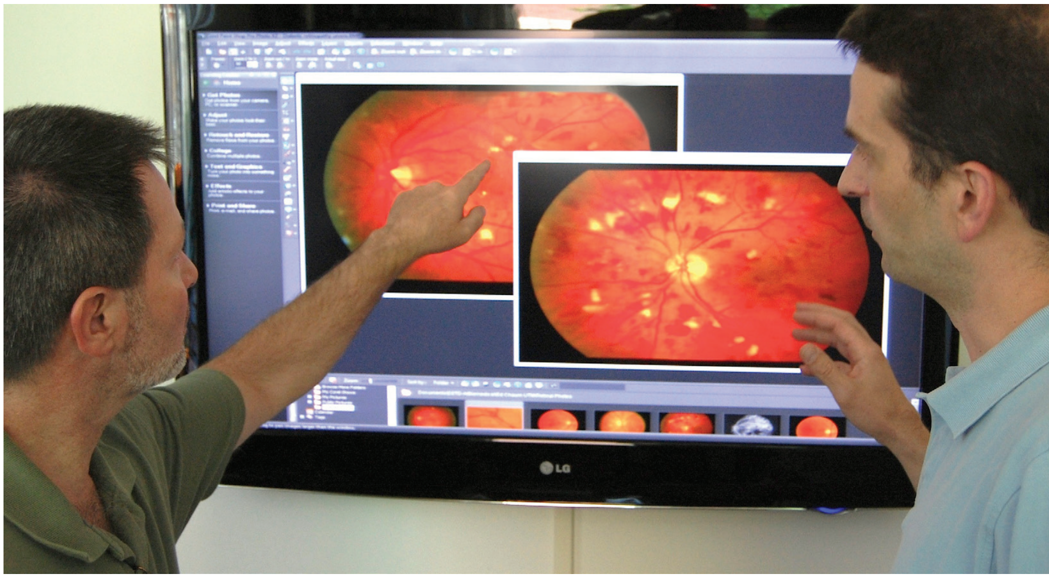
Pennycook and ORNL colleague Matthew Chisholm were joined by a team that included Sokrates Pantelides, Mark Oxley and Timothy Pennycook of Vanderbilt University and ORNL; Valeria Nicolosi at Oxford University; and Ondrej Krivanek, George Corbin, Niklas Dellby, Matt Murfitt, Chris Own and Zotlan Szilagyi of Nion Company, which designed and built the microscope. The team's Z-contrast STEM analysis is described in an article published in the March 25, 2010, issue of the journal *Nature*.

The team's new high-resolution imaging technique enables materials researchers to analyze, atom by atom, the molecular structure of experimental materials and discern their structural defects. Defects introduced into a material—for example, the placement of an impurity atom or molecule in the material's structure—are often responsible for the material's properties. The group analyzed a monolayer hexagonal boron nitride sample prepared at Oxford University and was able to find and identify three types of atomic substitutions: carbon atoms substituting for boron, carbon substituting for nitrogen and oxygen substituting for nitrogen. Boron, carbon, nitrogen and oxygen have atomic numbers, or Z values, of five, six, seven and eight, respectively.

The experiments were performed on a 100-kilovolt Nion UltraSTEM microscope optimized for low-voltage operation at 60 kilovolts. Aberration correction, in which distortions and artifacts caused by lens imperfections and environmental effects are computationally filtered and corrected, was conceived of decades ago but only in recent years made possible by advances in computing. Aided by the technology, ORNL's electron microscopy group set a resolution record in 2004 with the laboratory's 300-kilovolt STEM.

The recent advance comes at a much lower voltage for a reason. "Operating at 60 kilovolts enables us to avoid atom-displacement damage to the sample, which is encountered with low Z-value atoms above about 80 kilovolts," Pennycook says. "We could not perform this experiment with a 300-kilovolt STEM." Armed with the high-resolution images, materials, chemical and nanoscience researchers and theorists can design more accurate computational simulations to predict the behavior of advanced materials, which are key to meeting research challenges that include energy storage and energy-efficient technologies. Ⓡ

The team's new high-resolution imaging techniques enable analysis of the molecular structure of experimental materials.



ORNL's Ken Tobin and Tom Karnowski examine a computer automation method to aid in the diagnosis of diabetic retinopathy and other blinding eye diseases.

Measurement and the "circle" of research

"If you can't measure it, you're not doing science." The expression evolved to a large extent from the fact that the process of scientific inquiry is based on the ability to produce measurable and reproducible results. Thus it comes as no surprise that Ken Tobin, director of ORNL's Measurement Science and Systems Engineering Division, sees measurement playing an increasingly central role in the entirety of research performed at the laboratory. "I think of measurement science as an integral part of a 'circle' of research that connects fundamental and computational sciences," Tobin says. "Measurement systems are the key to translating observations from the physical world into data that can be analyzed by computational systems. To complete the circle, computational systems simulate 'virtual' new materials providing researchers with the insights they need to create these materials in the lab, which requires significant measurement and characterization capabilities." This process starts the cycle again: materials, measurement, computation, measurement and back to materials. Tobin believes the ability to accurately measure, characterize and control physical, biological, environmental or other engineered processes is critical to all of the work done at ORNL, regardless of whether the measurements involve analyzing new materials, calculating the impact of carbon in the environment or controlling the electric grid.

Tobin's division specializes in exploring and developing measurement systems that sample the physical world to produce high-fidelity and reliable data. The systems the researchers develop often extend the reach of existing technologies or create entirely new capabilities. "For example," Tobin says, "one of our projects that links basic science to applied research is our work in developing nanostructured surfaces." These unusual materials can be used for a range of applications, including producing surfaces with an amazing ability to repel water. These surfaces have practical applications in anti-icing, fabric coatings and novel sensors. Measurement science enters the picture when researchers are required to devise ways of determining how efficiently these materials accomplish their aims. "We have developed systems that can accurately measure a material's ability to repel water by looking at the contact angles of water droplets on surfaces in a variety of ways," Tobin explains, adding "we are also using the same kind of nanostructured materials to produce entirely new measurement devices."

ORNL researchers also use their electronics expertise to produce sophisticated and highly customized measurement systems. "The electronics for the Nuclear Materials Identification System have undergone quite a bit of evolution since we developed it in the 1990s," Tobin says. The instrumentation developed for the system enables technicians to make precisely timed measurements to scan containers to determine the presence of nuclear materials. ORNL scientists originally developed this system in support of the Strategic Arms Reduction treaties. Today the system is also used by the Department of Homeland Security in a range of applications, including air cargo examination and monitoring for highways, railways, ports and harbors.

In the biomedical area, Tobin's group has developed computed tomography systems to support mammalian genetics work. "When the project began several years ago, the idea was to be able to detect nonvisible manifestations of disease in animals using a high-throughput, high-resolution anatomic scanner. We made it possible for geneticists to take measurements from a large number of unique mice without having to destroy them," Tobin says. Recent spinoffs from the program include the development of functional imaging using single photon emission computed tomography (SPECT) to show how small animals metabolize glucose or incorporate protein.

Tobin sees measurement science playing an increasingly important role in the laboratory's research. "We're making inroads into new areas of measurement," Tobin says, pointing to microelectrical mechanical systems as an area in which his team is increasingly conducting research. The sensors can be used for a range of applications, from collision avoidance to instrumentation, for small modular nuclear reactors. The trend is toward integrating the sensors into wireless networks that communicate to a central control system. "This kind of comprehensive measurement and control system is an important aspect of what we are trying to achieve as we go forward in the measurement research area," Tobin says. "We continue to grow our research capabilities and generate output that supports the lab's energy mission, addressing new methods, instruments and integrated systems for energy efficiency, renewable energy, transportation, nuclear energy and nonproliferation technologies." Ⓡ

...and the WINNERS are...

Accomplishments of Distinction at Oak Ridge National Laboratory

Herbert A. Mook, Jr., has received the **Clifford G. Shull Prize** from the **Neutron Scattering Society of America** for his "outstanding contributions to the study of magnetism, superconductivity, and quantum phenomena in matter with neutrons." Since 1965, Mook has spent his career at ORNL, where he has expanded his neutron scattering research to investigate the interaction of magnetism and superconductivity. Among Mook's diverse range of experiments utilizing neutrons, he and collaborators have studied the nature of the magnetic structure and fluctuations in high-temperature superconductors using ORNL's High Flux Isotope Reactor.

Sergei V. Kalinin has received the **Burton Medal** from the **Microscopy Society of America** to honor his distinguished contributions to the field of microscopy and microanalysis.

The **Atom-by-Atom Analysis** work of **Stephen Pennycook**, **Matt Chisholm**, **Sokrates Pantelides**, **Mark Oxley**, **Timothy Pennycook** and their colleagues at **Oxford University** and the **Nion Company** was featured on the cover of the March 25, 2010 issue of ***Nature***.

Roger Stoller has been elected **Chairman of the Board of Directors** of the **American Society for Testing and Materials International**.

William Weber has been appointed by **Tennessee Governor Phil Bredesen** to the **Governor's Chair**, **University of Tennessee–ORNL, for Radiation Effects on Materials**.

Patricia Dreyer Parr has been elected **Chair** of the **Discover Life in America Board of Directors**.

Thom Mason and **Stephen E. Nagler** have been elected **Fellows of the Neutron Scattering Society of America**.

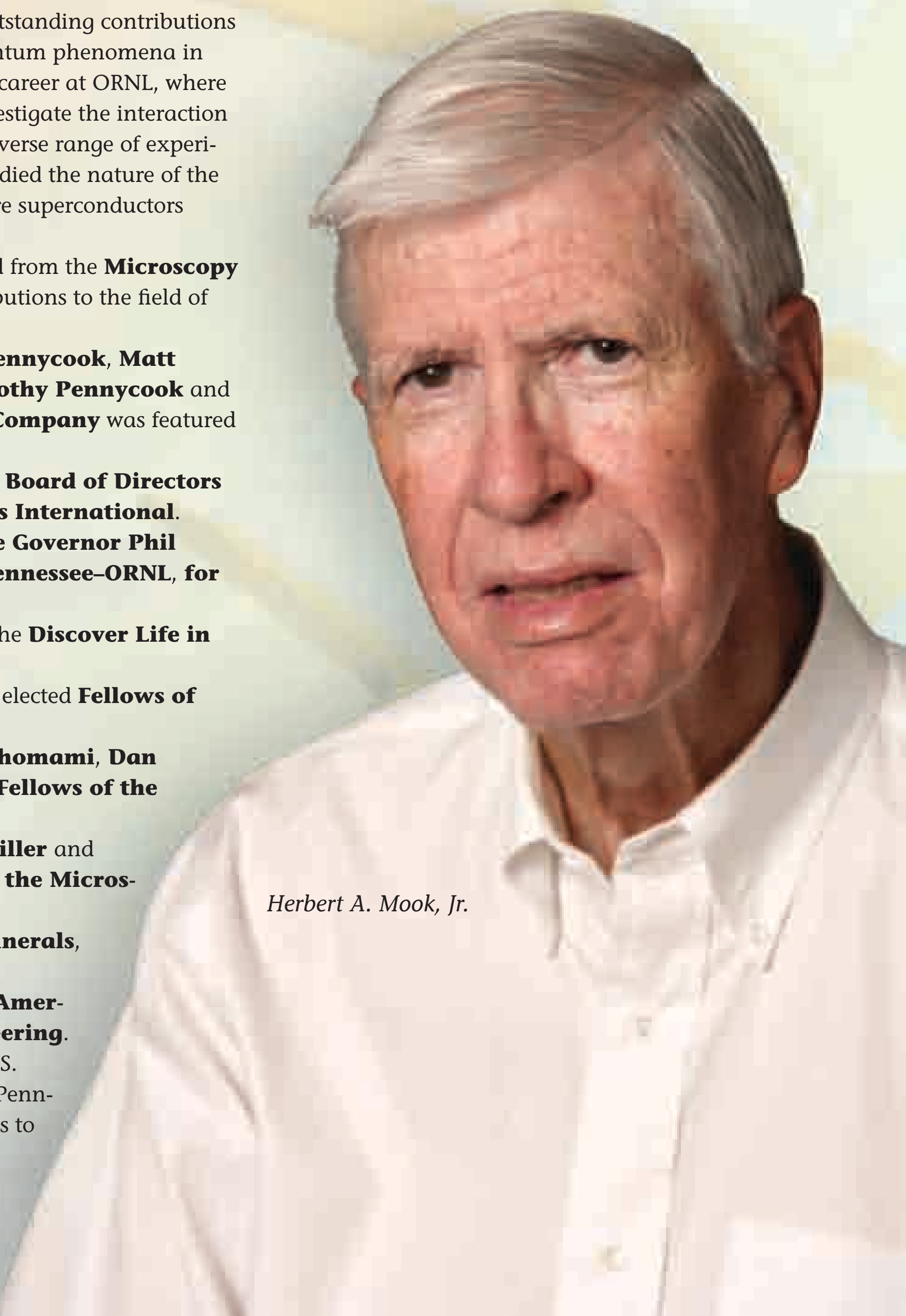
Matthew F. Chisholm, **Carl J. Gross**, **Bamim Khomami**, **Dan Shapira** and **Harm H. Weitering** have been elected **Fellows of the American Physical Society**.

Lawrence Frederick Allard, Jr., **Michael K. Miller** and **Stephen J. Pennycook** have been elected **Fellows of the Microscopy Society of America**.

Easo George has been elected a **Fellow of the Minerals, Metals and Materials Society.**

Mike Simpson has been elected a **Fellow of the American Institute for Medical and Biological Engineering**.

Robert A. Roboski has received an award from U.S. Immigration and Customs Enforcement, Philadelphia, Pennsylvania, in recognition of his outstanding contributions to counter-proliferation investigations.



Herbert A. Mook, Jr.

next issue

online extras

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Reference desk:

- Read journal papers on research described in this issue.

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