Oak Ridge National Laboratory

MANAGED BY UT-BATTELLE FOR THE U.S. DEPARTMENT OF ENERGY

Neutron Sciences

neutron review

OAK RIDGE NATIONAL LABORATORY

NEUTRON SCIENCES

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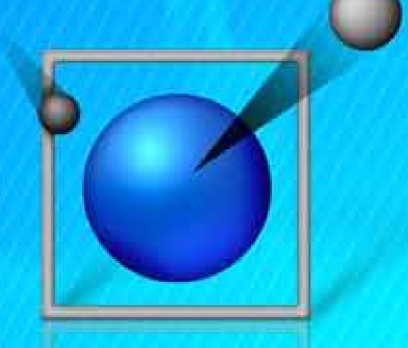
ORNL NEUTRON SCIENCES

NEUTRON REVIEW



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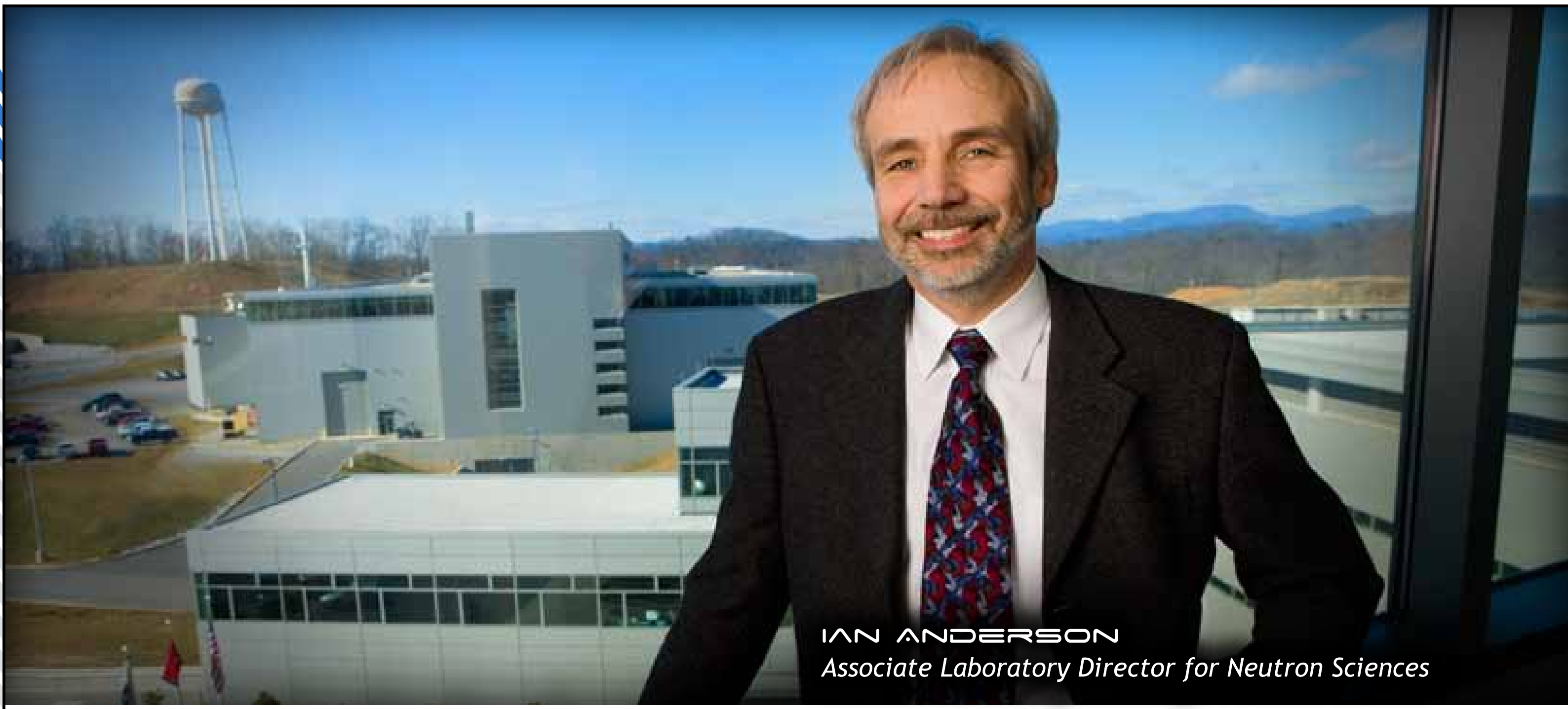
CONTENTS



Welcome

IT IS ALWAYS A PLEASURE AS WE COMPILE THE NEUTRON REVIEW MATERIAL TO SELECT THE HIGHLIGHTS THAT SHOWCASE THE DIRECTORate's scientific productivity and accomplishments. This review covers almost two years of activity and marks the fifth year of joint operation of the Spallation Neutron Source and the High Flux Isotope Reactor at Oak Ridge National Laboratory.

A particularly exciting research area is the new class of iron-based superconductors, and both facilities have been at the forefront of the activity with a number of leading results emanating from our instruments. In this report you will also find scientific results ranging from sorption of CO_2 in coal to phonon vibrations in thermoelectric materials to the molecular structure of switchgrass. The numbers of research papers and types of research conducted continue to grow and diversify, as we now have 14 instruments at SNS and 14 at HFIR either available to users or in commissioning. In the last proposal review round, more than 700 research proposals were submitted for a six month period of beam time. The demand is high and increasing rapidly.

The key to addressing this high demand is the very high reliability of our neutron sources, both of which are running exceptionally well. SNS reliability for FY 2010 was 88% at power levels of 1 MW; to date in FY 2011, we are achieving 92%! HFIR completed seven cycles in FY 2010 for a total of 14,293 MW days and the outstanding predictability remained at 98.8%. You'll find summaries of our many operational and technological achievements in this report, ranging from sample environment and detector developments to data acquisition and analysis.

Of particular note is the unprecedented deluge of data from the SNS instruments—most instruments are producing many tens of gigabytes per day, and the total volume of stored data has surpassed 50 terabytes. Data production is roughly doubling in each run cycle. Obviously our users can't take all these data home, so they use our remote access systems to view, manipulate, and analyze data. The Neutron Sciences Data Portal systems were hosting as many as 130 users a day and 71,000 computing jobs a month by the end of 2010. That's a record for any neutron facility.

Our contributions to neutron science education included the National School on Neutron and X-Ray Scattering (co-hosted with Argonne National Laboratory) and the Dynamics of Soft Matter Workshop at the annual meeting of the Materials Research Society, which resulted in a new book in the Springer series Neutron Scattering Applications and Techniques. In addition, a group of Neutron Sciences staff developed and went on the road with the "SNS simulator," a hands-on display used to educate middle school kids about neutron science.

As you read the report, share with me the excitement of a growing, vibrant center for the study of materials at the atomic scale.

Ian Anderson

Year in Review

DURING 2010, THE NEUTRON SCIENCES DIRECTORATE FOCUSED ON PRODUCING WORLD-CLASS SCIence, while supporting the needs of the scientific community. As the instrument, sample environment, and data analysis tools at High Flux Isotope Reactor (HFIR) and Spallation Neutron Source (SNS) have grown over the last year, so has promising neutron scattering research. This was an exciting year in science, technology, and operations.

HFIR and SNS Experiments Take Gordon Battelle Awards for Scientific Discovery

Battelle Memorial Institute presented the inaugural Gordon Battelle Prizes for scientific discovery and technology impact in 2010. Battelle awards the prizes to recognize the most significant advancements at national laboratories that it manages or co-manages.

Two of the five Gordon Battelle prizes for scientific discovery were presented to HFIR and SNS teams for the discovery of element 117, which used isotopes created at HFIR, and for groundbreaking studies of iron-based superconductors conducted on triple-axis spectrometers at HFIR and the Wide Angular-Range Chopper Spectrometer (ARCS) at SNS.

ORNL Director of Strategic Capabilities Jim Roberto, who helped initiate the experiment, at the celebration of the discovery of element 117. "Without the berkelium target, there could have been no experiment," Roberto says.

Discovery of Element 117

As part of an international team of scientists from Russia and the United States, HFIR staff played a pivotal role in the discovery by generating the berkelium used to produce the new element. A total of six atoms of "ununseptium" were detected in a two-year campaign employing HFIR and the Radiochemical Engineering Development Center at Oak Ridge National Laboratory (ORNL) and the heavy-ion accelerator capabilities at the Joint Institute for Nuclear Research in Dubna, Russia.

The discovery of the new element expands the understanding of the properties of nuclei at extreme numbers of protons and neutrons. The production of a new element and observation of 11 new heaviest isotopes demonstrate the increased stability of super-heavy elements with increasing neutron numbers and provide the strongest evidence to date for the existence of an island of enhanced stability for super-heavy elements. See p. 19 for more.

Studies of Iron-Based High-Temperature Superconductors

ORNL applied its distinctive capabilities in neutron scattering, chemistry, physics, and computation to detailed studies of the magnetic excitations of iron-based superconductors (iron pnictides and chalcogenides), a class of materials discovered in 2008. ORNL team members worked with researchers from Argonne National Laboratory and the ISIS facility at Rutherford-Appleton Laboratory in the UK.

This research is yielding new insights into the relationship between magnetism and superconductivity and has established several key features of this family of high-temperature superconducting (HTS) materials: the maximum magnetic field at which they can function, the nature of the electrons involved in the superconductivity, the dependence of the properties upon chemical substitution, and the character of the magnetic fluctuations in the material. The results suggest that despite important differences between these materials and the HTS copper oxides, a universal mechanism may be responsible for the unconventional superconductivity.

HTS materials conduct electricity without resistance at temperatures that make them usable in practical applications and thus have enormous potential for energy efficiency. The emergence of the iron-based superconductors has rejuvenated the field of high-temperature superconductivity. See p. 16 for more.

Coal Sequestration Research: A New Home for Greenhouse Gases

One possibility for slowing down the increasing levels of carbon dioxide (CO_2) in the atmosphere is to capture the gas in natural underground features such as coal seams. Critical to the feasibility of this technology is determining how much CO_2 can be stored, no method for which has been found—until now.

Researchers working at HFIR and SNS have developed unique high-pressure cells that correspond to underground conditions in coal seams with a depth down to 10 km below sea level. Novel interpretation of their data allows them to "look inside" pores and obtain information about how well each different size of coal pore can adsorb CO_2. Further experiments demonstrate that small pores work as "molecular pumps" that condense confined greenhouse gases into liquid. This continuing research promises new possibilities for dealing with the pervasive issue of global warning. See p. 34 for more.

Accelerator Reliability Passes 92%

In December 2010, SNS set a new record for itself when the accelerator ran at 1 MW with 100% reliability.

Annual accelerator reliability has climbed from 66% in 2007 to an average of more than 92% to date. Sustained operation has been achieved with more than 98% reliability over a one-week period and with more than 95% reliability over a one-month period.

"This is a remarkable achievement for such a new accelerator, especially considering it is operating in a pulsed mode at sustained high power (1 MW)," says Accelerator Physics Group leader John Galambos.

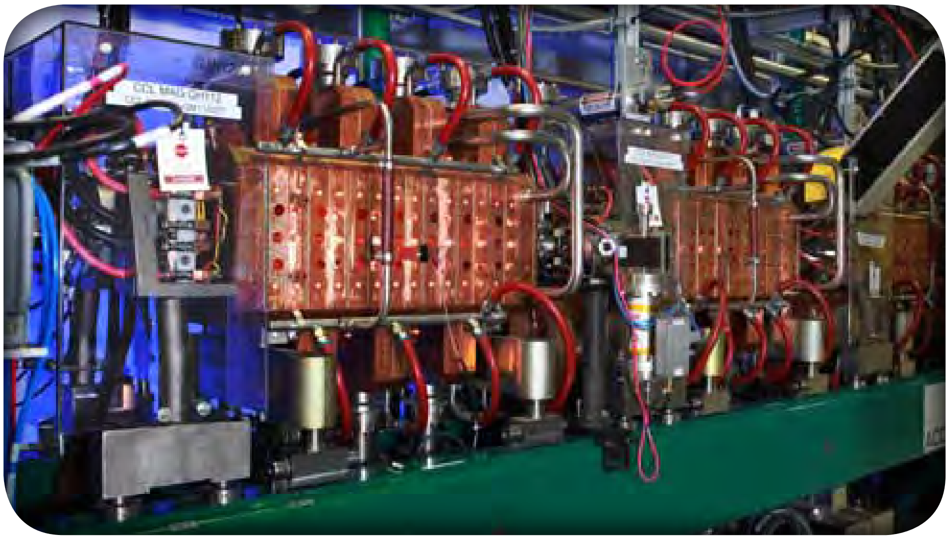
"All this adds up to good news for the neutron users. Not only do they have access to the brightest pulsed neutron source in the world, but the facility is also becoming a world leader in the equally important arena of reliability," Galambos says. "Because the typical user spends only a few days at a facility, it is vital to keep the accelerator on as much as possible so that users can concentrate on their experiments without interruptions from accelerator down time." See p. 44 for more.

Target Performance Exceeds All Expectations

The mercury target used at SNS is the first of its kind. During the design and planning for SNS, many people were skeptical that the target would work. In 2010, it was confirmed that the target was working not only well but much better than anyone would have imagined.

During the summer of 2010, what was only the second target to have been installed since the SNS start up in 2006 was replaced. That target had endured a full year of operation with more than 1250 hours of proton beam operation above 900 kW.

This performance exceeded all expectations. The energetic protons coming from



Coupled-cavity section of the SNS linear accelerator.

the SNS accelerator do permanent damage to the target casing, and in the planning stages of SNS, the resiliency of the unique target design was a major concern. At one point, design alternatives were considered.

"We have established that the target can withstand powers in the range of 1 MW for half a year's worth of operation," says John Haines, director of the Neutron Facilities Development Division. "We are quite pleased with this outcome, which confirms the 'wisdom' (some might say luck) of deciding to go with a mercury target." See p. 48 for more.

Helium-3 detector.

Changing the World of Data Acquisition

Researchers at SNS are starting to benefit from event-based data analysis. Event data mode captures and stores an individual data set for every single neutron that strikes a detector—precisely when and where the neutron is detected. This technique provides numerous advantages over traditional methods.

Event data mode allows researchers to process their data at the highest resolution possible with no loss of data. This method of data collection provides a much more efficient way for users to gather data and get the most from their beam time. See p. 46 for more.

New Laboratories for Users

The HFIR and SNS user communities continue to grow dramatically. In 2010, HFIR hosted 862 users and SNS 796, outpacing projections for both facilities. To meet the needs of those users, a new complex of 13 laboratories is now open for users at SNS. The labs provide a controlled environment for preparing and testing materials before they go on the beam line. The labs were built with overhead utilities and mobile furniture, allowing staff to easily reconfigure the layout of equipment and quickly change an experiment's setup as needed. See p. 55 for more.

Innovative Detectors Provide Relief from Helium-3 Shortage

Helium-3 (^{3}He) has been the gas of choice for gaseous detectors since the early days of neutron science. About two years ago, detector scientists worldwide faced the reality that stockpiles of ^{3}He are dwindling rapidly, while demand for it has risen by a factor of five.

The Neutron Sciences Detectors Group has developed two new types of detectors that don't rely on ^{3}He: the Anger camera and the wavelength shifting fiber neutron detector, both of which use lithium (^{6}Li). Not only do these detectors reduce the need for ^{3}He, but also their performance has surpassed traditional detectors.

The ORNL team has installed huge Anger camera arrays at two SNS instruments (SNAP and TOPAZ), and SNS now has 10 times as many Anger cameras as any other facility in the world. Those arrays have performed extremely well, achieving higher-rate capacity and higher resolution than has ever been achieved with a mass-produced detector system. See p. 45 for more.

New Education and Outreach Initiatives

A lot of energy went into education and outreach efforts in 2010. A milestone was the opening of the Joint Institute for Neutron Sciences, (JINS) ideally located on the SNS site, with easy access to HFIR and the Center for Nanophase Materials Sciences. Co-founded by ORNL and the University of Tennessee, JINS provides modern facilities and

Visitors at the SNS simulator can press a button to see "spallation" at the display's target area.

collaborative opportunities for multi-institutional research teams.

In addition to our regular activities with workshops and students, we participated in two programs for teachers, Academies Creating Teacher-Scientists Professional Development Program and the nationwide program Siemens Teachers as Researchers. These programs give teachers hands-on experience with neutron science that they can take back home to their students.

Communications Group staff created the "SNS simulator," an interactive display designed to teach middle school kids and teachers about neutron science. The display made appearances at three events, including the inaugural National Science and Engineering Festival in Washington, D.C. Requests for participation in other events are pouring in. See p. 64 for more.

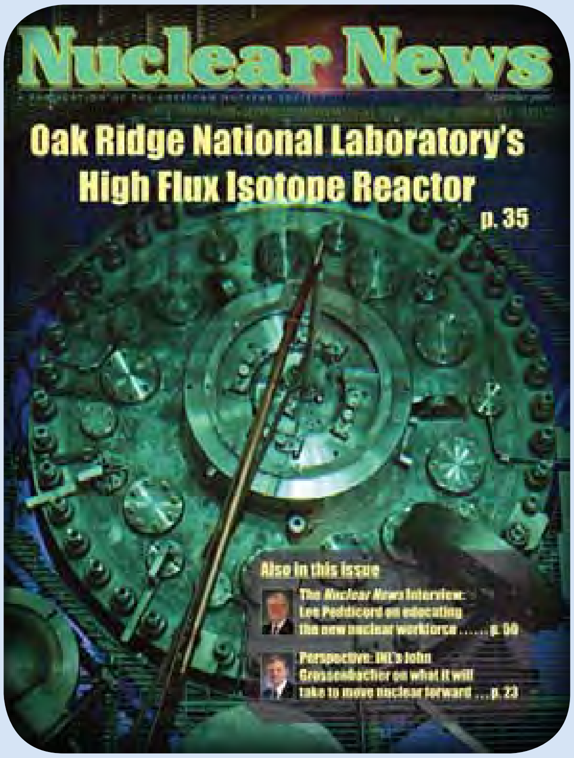
Operations Beyond Expectations

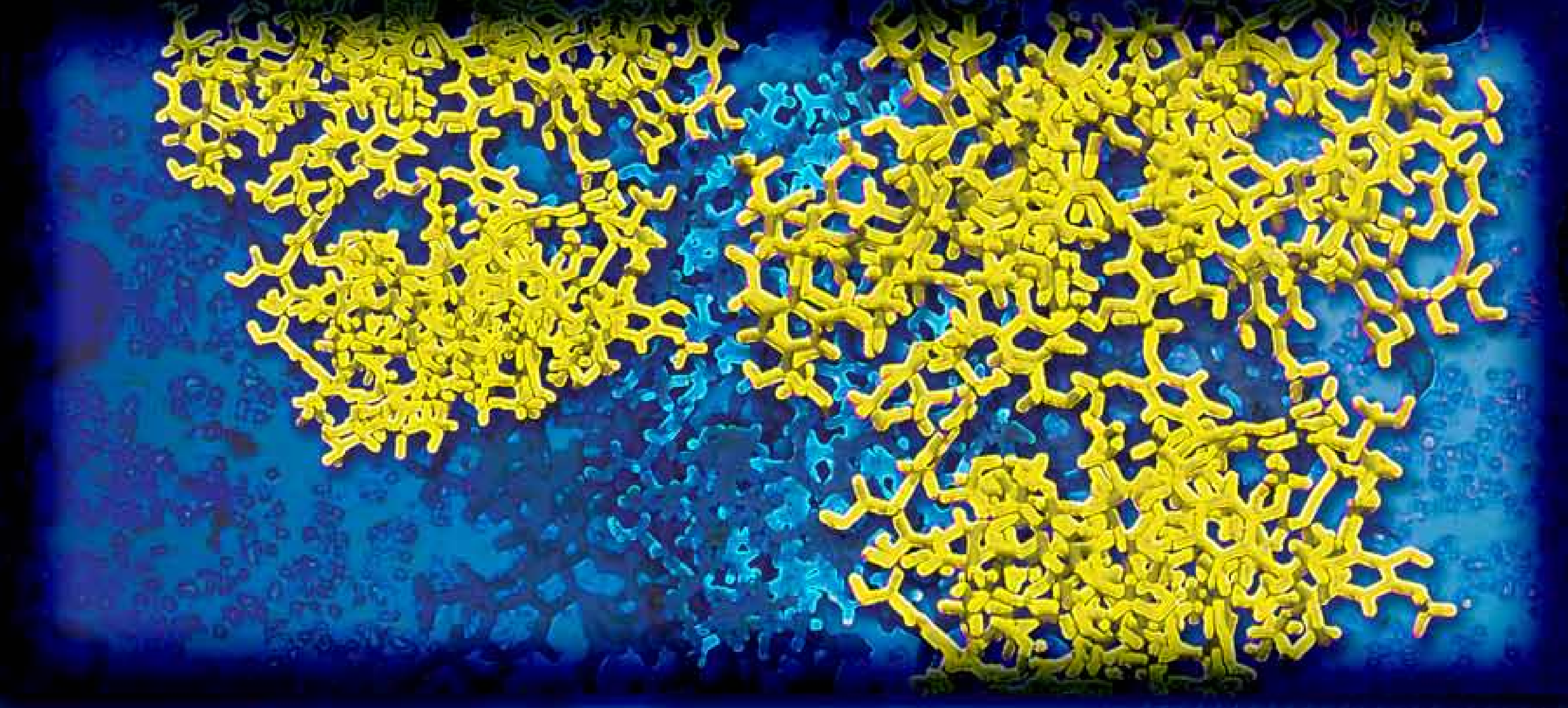
SNS operations progress was significant in 2010, the fourth full year of operation. Fiscal year operational goals were exceeded in every area with the delivery of 4226.3 neutron production hours (7.5% over goal), 3431.4 MW hours (5.4% over goal), and 5265 total operating hours (almost 10% over goal). After achieving 1 MW of beam power on target in 2009, SNS routinely operated between 0.8 and 1 MW during 2010.

HFIR also exceeded its production and reliability goals for FY 2010. Predictability for the year was 98.9%, seven cycles were completed, and MW days totaled 14,293. In addition, HFIR produced 43 commercial and medical isotopes and conducted 387 materials irradiations and 233 neutron activation analyses. It was the third full year of HFIR operation with the cold neutron source.

Scientific output during 2010 resulted in more than 200 journal articles produced by scientists working at SNS and HFIR. A significant portion of those were in some of the most prestigious journals in their respective fields.

Complete lists of these publications are available at neutrons.ornl.gov/media/pubs/2010-published.shtml.





ABOUT US

ORNL Neutron Sciences

TWO OF THE WORLD'S MOST ADVANCED NEUTRON SCATTERING RESEARCH FACILITIES—THE SPALLation Neutron Source and the High Flux Isotope Reactor—are located at ORNL. The two attract scientists from all over the world to conduct basic scientific research.

Funded by the U.S. Department of Energy (DOE) Office of Basic Energy Sciences, SNS and HFIR are national user facilities managed by the ORNL Neutron Sciences Directorate. The Neutron Sciences vision is to provide unprecedented capabilities for understanding the structure and properties of materials across the spectrum of biology, chemistry, physics, and engineering and to stay at the leading edge of neutron science by developing new instruments, tools, and services.

The main goal for the directorate is excellence in science, and all of its activities support this purpose. Through reliable operation and continual development, Neutron Sciences strives to capitalize on the capabilities of two of the world's highest-flux neutron beams, one pulsed and one continuous. The two facilities have a common user program and integrated operations. In addition to serving its users, Neutron Sciences is focusing efforts on reaching out to the scientific community to educate current and future scientists about the benefits of using neutron scattering for their research.

Christina Hoffmann, lead instrument scientist, and Matt Frost, scientific associate, work on TOPAZ, a new single-crystal diffractometer at SNS. TOPAZ will greatly expand the range of materials that can be studied in biology, chemistry, earth sciences, materials, and solid-state physics.

SNS was designed from the beginning to be upgraded to 3 MW of power and to accommodate a second target station to expand the scientific capabilities of the complex.

A power upgrade project is in the works that will increase beam energy by 30% from 1.0 to 1.3 GeV. A reference design concept for the second target station has been developed.

The new station will provide 1 MW at 20 Hz, and each pulse will use the full 1-ms-long pulse directly from the SNS linear accelerator. An optimized instrument suite on this target station will complement the capabilities available at the first target station. These additional instruments will provide more than an order-of-magnitude performance improvement for broad areas of forefront science and will open totally new areas to scientific exploration with neutrons. When most of its instruments are operational, the second target station will nearly double the scientific output of the SNS facility.

Contact: Kent Crawford, crawfordrk@ornl.gov

Spallation Neutron Source

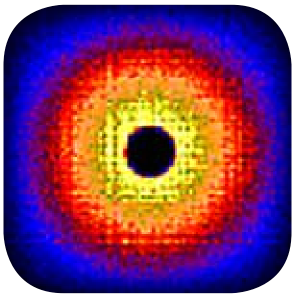
SNS IS AN ACCELERATOR-BASED NEUTRON SOURCE THAT PROVIDES THE MOST INTENSE PULSED NEUTRON BEAMS in the world for scientific and industrial research and development. SNS will eventually have a suite of 25 instruments, the best of their kind, that will enable scientists to make more detailed examinations of smaller samples of materials than ever before possible.

High Flux Isotope Reactor

THE 85-MW HFIR PROVIDES ONE OF THE HIGHEST CONTINUOUS FLUXES OF NEUTRONS OF ANY RESEARCH REACTOR in the world, and its cold source is the brightest in the world. HFIR has four missions: neutron scattering research (the focus of this report), isotope production, materials irradiation, and neutron activation analysis. HFIR has 15 instruments either in operation or planned, including two cold-source instruments.

Complementary ORNL Facilities

RESEARCH CAPABILITIES AT SNS AND HFIR ARE ENHANCED BY THE PROXIMITY OF OTHER ORNL USER facilities, most with the same access and training requirements. Major user facilities at ORNL include the following:



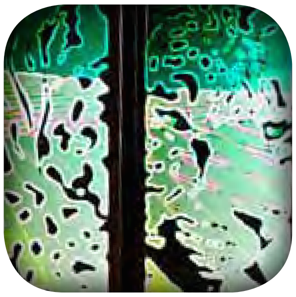
CSMB: Microemulsion droplet measured on the Bio-SANS instrument.

The Center for Structural Molecular Biology (www.csmb.ornl.gov) operates the HFIR Bio-SANS. It develops methodologies for the structural molecular biology research community and computational tools to analyze and interpret SANS data.

The Bio-Deuteration Laboratory (www.csmb.ornl.gov/Bio-DeuterationLab.html) is designed for in vivo production of hydrogen/deuterium-labeled biomacromolecules. It supports cloning, protein expression, purification, and characterization of deuterium-labeled biological macromolecules.

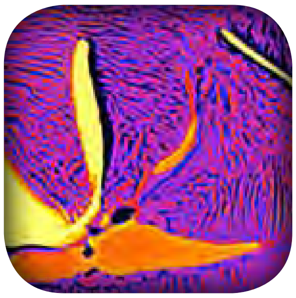
CNMS: Gallium ball-Si crystal-SiO$_x$ nanowire octopus.

The Center for Nanophase Materials Sciences (www.cnms.ornl.gov) provides a complete suite of unique capabilities for studying nanoscale materials and assemblies.



NCCS: Cray "Jaguar" supercomputer.

The National Center for Computational Sciences (www.nccs.gov) hosts the Cray "Jaguar" supercomputer, the most powerful computing system in the world with a peak power of 2.33 petaflops (2.33 quadrillion floating point operations per second); Kraken, the world's third-fastest system that clocks 1.17 petaflop; and other computers among the world's most powerful.



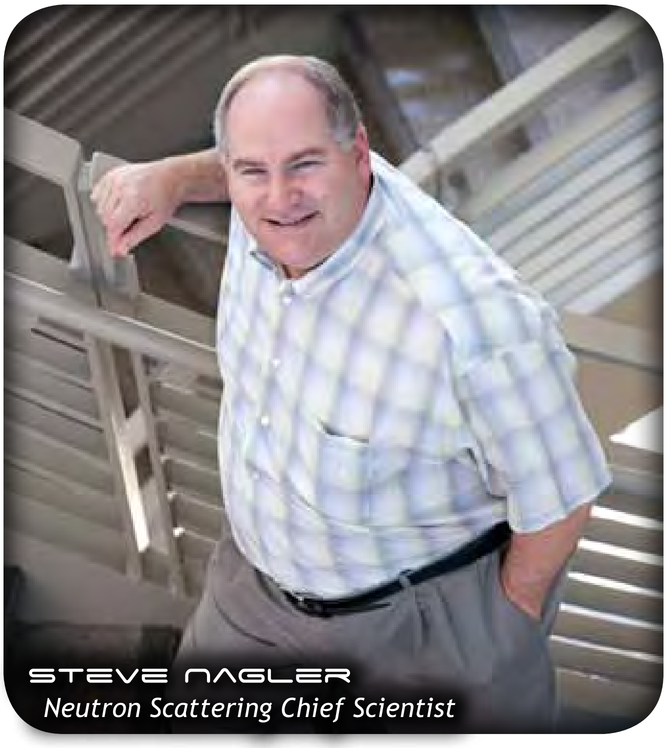
SHaRE: magnetically processed cast iron.

The Shared Research Equipment User Facility (www.ms.ornl.gov/share) offers a suite of advanced instruments and expert staff scientists for micrometer- to-nanometer-scale characterization of materials in several research areas: transmission and scanning electron microscopy, atom probe tomography, x-ray photoelectron spectrometry, and dual beam focused ion beam and ultramicrotomy specimen preparation and support.

HTML: environmental testing.

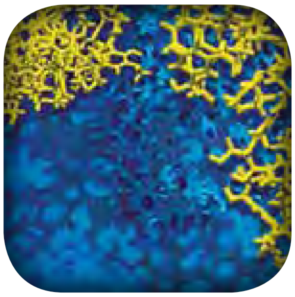
The High Temperature Materials Laboratory (www.html.ornl.gov) helps solve materials problems that limit the efficiency and reliability of automotive systems. The center's instruments can characterize the structural, chemical, physical, and mechanical properties of materials at the nanoscale and microscale over a wide range of temperatures and pressures.

SCIENCE HIGHLIGHTS

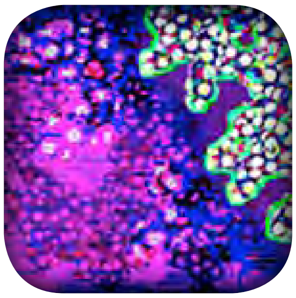


STEVE NAGLER
Neutron Scattering Chief Scientist

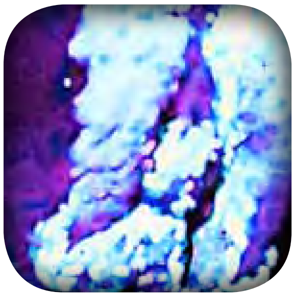
Superalloys



Biomass



Biosynthetics



Extreme Environments

From the Neutron Scattering Chief Scientist

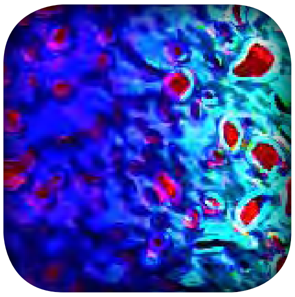
DURING THE PAST YEAR THE SCIENCE CARRIED OUT AT ORNL’S NEUTRON FACILITIES HAS CONTINued to build, flourish, and diversify. This is visible literally in the striking neutron images produced from research probing the flow of vehicle emission gases, lithium ions in batteries, and water motions in soil by Hassina Bilheux and her colleagues. The pictures are easy for anyone to understand and are often quite visually compelling. It’s hard to imagine just where imaging techniques will be taken in the coming years, but it is guaranteed to be fascinating news.

Other research groups present their data in four-dimensional reciprocal-frequency space, which although harder to explain to one’s grandmother, contains equally important and interesting science. Olivier Delaire dubs his measurements “single-crystal reciprocal space tomography” and, using a combination of neutron measurements and high-powered computer calculations, has been able to make notable progress in understanding some of the fundamental science behind thermoelectric materials. This research ultimately could pay off in the form of improved energy efficiency in households and industry.

Relevance to energy has been a consistent theme in other research too. Small-angle neutron scattering (SANS) has been particularly instructive and has helped investigate better ways of producing biomass on the one hand and the possible use of underground coal to sequester CO_2 on the other. Some advanced biological applications of SANS included new detailed determinations of the structures of viruses and an investigation of the means of distributing proteins in biomineralized silica.

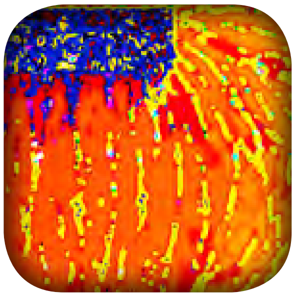
The penetrating power of neutrons makes them ideal for characterizing large industrial components and provides a unique method of assessing wear and tear in the form of internal stresses. The results provide information that is essential for economics and safety studies for many different applications. An intriguing application of the VULCAN instrument was examination of superconducting cables used for the central solenoid in the international fusion project ITER. VULCAN is enabling a determination of the mechanical effect of the electromagnetic Lorentz force on the massive 1 inch diameter cables used in the solenoid. The NSRF-2 facility at HFIR has also been used for stress measurements relevant to industries as varied as transportation, construction, and nuclear power.

Superconductors

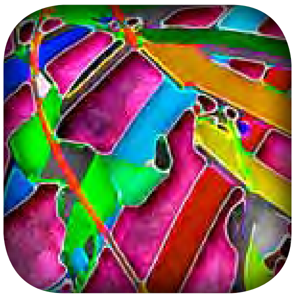


Nanomaterials

Nanoparticles



Magnetism

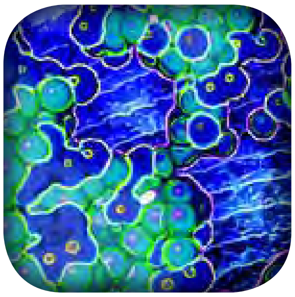


Biomolecules

Catalysts

Biotechnology

Polymers



Copolymers

Proteins

Biofuels

Research using the high-pressure instrument SNAP has looked at the structure of clathrate hydrates, cage-like materials that can store normally gaseous materials like methane at extremely high density. A better understanding of these materials could provide a high payoff in many different areas. Payoff in the form of better fuel cells motivated research on ionic liquids using the high-resolution BASIS instrument. Here the motion of atoms is intimately linked to the performance of real devices.

Frontier research in hard condensed matter physics remains robust and dynamic, with interesting advances in multiferroic materials, magnetism, and novel superconductors at both HFIR and SNS. The striking data produced at the Cold Neutron Chopper Spectrometer show why this instrument is in such high demand.

Finally, it's not every day that new elements are discovered, and the critical role of HFIR in producing element 117 is one of the exciting accomplishments of the year. I hope that you enjoy reading about these and other advances, as we look forward to even more exciting things in the year to come.

Steve Nagler, Neutron Scattering Science Division
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Neutron Scattering Continues as a Vital Tool in Superconductivity Studies

Neutron scattering shows magnetic excitation mechanism at work in new materials.

IN 2008, THE TOTALLY UNEXPECTED DISCOVERY OF A NEW CLASS OF SUPERCONDUCTORS, THE IRON PNICTIDES, SET OFF A FEVERISH international effort to understand them. The instruments and scientists at HFIR and SNS are leaders in exploring these exotic materials, scanning the subatomic details of their structures and magnetic properties.

Several key discoveries about the iron-based superconductors (Fe SCs) have emerged from research conducted at ORNL's neutron science facilities. Mark Lumsden and Andy Christianson of ORNL and Pengcheng Dai of ORNL and the University of Tennessee led early neutron scattering studies of the pnictides. Their work has revealed important details about the magnetic order of the parent compounds and its correlation with the emergence of superconductivity.

The Fe SCs are likely to have a broad range of practical uses, but their fascination for researchers is their fundamental physics. What they offer is a research platform more amenable to tinkering and more accessible to theory than the copper-based cuprate superconductors. The pnictides are structurally simpler and more chemically flexible than the cuprates, and a greater variety of Fe SCs can be synthesized, note Lumsden and Christianson. In addition, "theorists have more of a handle on the iron pnictides than the copper oxides," Dai says. "Our hope for the iron-based superconductors is that, long-term, by understanding them, we will understand the cuprates and all the unconventional superconductors."

Experimental tools available now—time-of-flight chopper spectrometers, position-sensitive detectors—were unknown when the cuprates were discovered, Dai notes. Measuring spin waves of up to 300 meV, routine now on instruments such as SNS's ARCS and SEQUOIA, was impossible only a few years ago, he says. Determining the exchange coupling of the cuprates took 15 years; doing the same for the iron pnictides took only a year or so because of the availability of powerful inelastic spectrometers.

Pengcheng Dai (left) and instrument scientist Doug Abernathy at ARCS.

Dai ticks off four main things neutron scattering has revealed about superconducting iron compounds since 2008: The parent iron compounds exhibit antiferromagnetic order, as in the cuprates. The effective exchange coupling is about 50 meV, less than in the cuprates. The nearest-neighbor exchange coupling is strongly anisotropic. And the next-nearest neighbor coupling is similar among the pnictides and the chalcogenides, two different classes of Fe SCs.

Also well established is that long-range magnetic order and superconductivity tend not to coexist. "It's clear that you need to get rid of long-range magnetic order, or at least suppress it, before superconductivity evolves," Lumsden says.

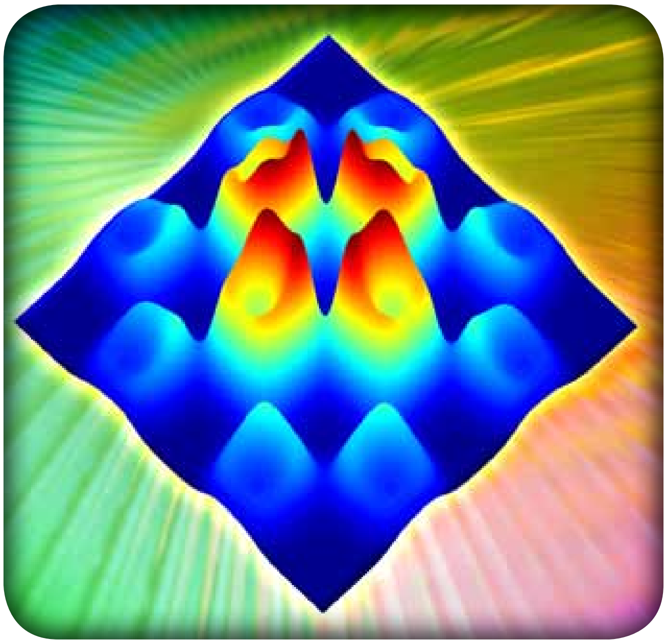
The lessons learned are mostly the basics, Christianson says. "We now know a lot about crystal structures. We know which materials we can make in this family that are superconducting and which are not. We know the basic magnetic properties, how these materials magnetically order, what the spin excitations look like. We know what the wave vector is in almost all cases where interesting magnetic behavior is occurring."

What are experiments on the Fe SCs contributing to the understanding of unconventional superconductivity? "Essentially, what we have learned about high-temperature superconductivity is that regardless of the material, the superconductivity always seems to be near an antiferromagnetic phase," says Dai. "We've learned that in the cuprates, in the case of heavy fermion superconductors, and now we've seen it in the case of iron-based superconductors."

Dai also notes the correlation between exchange coupling and the highest temperature at which superconductivity emerges in a material. That holds true for cuprate, pnictide, and heavy fermion superconductors. "So you have a whole span of materials. You can say this is all accident, but it may reveal some intrinsic features of the materials."

Big questions remain. Chief among them are the nature of the electron pairing symmetry and whether the magnetism is itinerant or local, say Lumsden and Christianson. Also, the entire magnetic spectrum, from zero energy to 300 meV, needs to be mapped for an Fe SC to see when it becomes superconducting and how the spin excitations evolve, Dai says. "From that, one can potentially calculate whether magnetic excitations have sufficient energy to drive superconductivity."

The recent discovery that iron selenide doped with potassium becomes superconducting is highly significant in the exploration of unconventional superconductivity, Dai notes. A key difference between cuprates and Fe SCs is that the parent compounds of the latter are metals. However, iron selenides doped with potassium or rubidium are insulators, like the cuprates. "This new class of materials could throw the thinking of the last three years into a tailspin. They hold the key to addressing some of the key debates."



This image depicts part of a spectrum of magnetic fluctuations in an iron-based superconductor measured using neutron scattering. Their form suggests a universal mechanism for the origin of superconductivity in both copper oxide and iron-based superconductors.

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Structure and Magnetic Order in Iron-Based Superconductors

Important clues to the mystery of superconductivity.

NEUTRON SCATTERING EXPERIMENTS AT HFIR, NIST, AND THE JAPAN ATOMIC ENERGY AGENCY were among the many neutron studies helping to clarify the role of magnetism in the unconventional superconductivity of the new iron-based pnictides. A recent elastic neutron scattering study at HFIR, led by H.-F. Li of Ames Laboratory, focused on the structural and magnetic phase transitions in a high-quality single crystal of the layered oxypnictide superconductor LaFeAsO. Previous studies with polycrystalline materials had provided important insights into the transitions of the parent compound LaFeAsO, but questions remained about the complexity of iron chemistry and its effect on the structural and magnetic transitions.

The experiments conducted by Li's team determine the magnetic form factor of the iron ions in this compound and suggest that the oxidation state of iron in LaFeAsO is close to that of Fe^{2+}. The iron magnetic moment is approximately 0.8 μ_B, about twice as large as the original value reported from the powder measurements but still much smaller than the 4 μ_B expected from a localized model. This new study also clarified that the transformation from a tetragonal (T) to orthorhombic (O) structure, which precedes the transition to a magnetically ordered state, occurs in two steps. The authors contend that the O and T structures coexist dynamically between T_S and T_P. Their coexistence could be related to a recently proposed nematic spin phase in the iron pnictides.

A study led by K. Matan, University of Tokyo, focused on the spin dynamics of the electron-doped material $Ba(Fe_{1-x}Co_x)_2As_2$ at cobalt concentrations corresponding to (1) the nonsuperconducting parent compound (x=0), (2) the optimally doped and overdoped superconducting compounds (x=0.06, 0.14), and (3) the "heavily overdoped" nonsuperconducting compound (x=0.24). A striking similarity was seen between the magnetic fluctuations in the paramagnetic state of the parent compound and those in the normal state of the optimally doped compound. In the overdoped superconducting compound, the magnetic excitations show a gap-like behavior, possibly related to a topological change in the hole Fermi surface, which resembles that of overdoped cuprate superconductors. This magnetic signal is completely suppressed in the heavily overdoped regime, where superconductivity disappears.

Results support the view that magnetism and superconductivity are strongly correlated and that differences in the spin dynamics at different doping levels reflect changes in electronic band structure.

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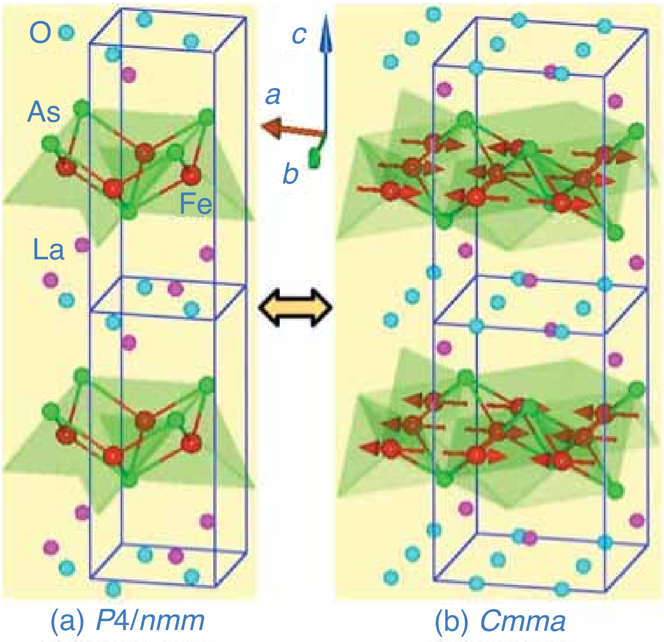

(a) *P4/nmm* (b) *Cmma*

Crystal structures above T_S (a) and below T_P (b). The structure below T_P is antiferromagnetic, which results in the doubling of the unit cell as shown in (b). The study by Li et al. suggests that these two structures coexist dynamically at temperatures $T_S>T>T_P$.

Discovery of New Chemical Element 117

Ununseptium fills in the missing element in row 7 of the periodic table.

A US-RUSSIAN TEAM, INCLUDING SCIENTISTS AND ENGINEERS FROM ORNL, USED ISOTOPES CREATED AT HFIR to discover a new chemical element. Discovered in April 2010, Z=117 is the most recent addition to the periodic table. A total of six atoms of “ununseptium” were detected in a two-year effort employing HFIR and the Radiochemical Engineering Development Center at ORNL and the heavy-ion accelerator capabilities at the Joint Institute for Nuclear Research and the Research Institute of Atomic Reactors in Russia.

ORNL team members included U.S. project manager James B. Roberto, Krzysztof Rykaczewski, D. E. Benker, J. G. Ezold, C. E. Porter, and F. D. Riley. The team also included researchers from Lawrence Livermore National Laboratory, Vanderbilt University, and the University of Nevada–Las Vegas.

The discovery won the researchers a Gordon Battelle prize for scientific discovery, announced on January 31, 2011 (See “Year in Review,” p. 5).

The two-year experiment began at HFIR with a 250-day irradiation to produce 22 mg of berkelium. This was followed by 90 days of processing at Oak Ridge to separate and purify the berkelium, target preparation at Dimitrovgrad, 150 days of bombardment at one of the world’s most powerful heavy ion accelerators at Dubna, data analysis at Livermore and Dubna, and assessment and review of the results. The entire process was driven by the 320-day half-life of the berkelium target material.

The experiment depended on the availability of special detection facilities and dedicated accelerator time at Dubna, unique isotope production and separation facilities at Oak Ridge, and distinctive nuclear data analysis capabilities at Livermore.

Element 117 was the only missing element in row seven of the periodic table. “It fills in the gap and gets us incrementally closer than element 116—on the edge,” says Ken Moody, one of the Livermore collaborators and a long term veteran of superheavy element (SHE) research. The researchers are still looking for relatively stable SHEs. An “island of stability” (proton and neutron numbers with longer lifetimes) is expected somewhere nearby. “The experiments are getting harder, but then I thought we were done 20 years ago.”

HFIR fuel element. In the center is the “target basket,” which contains 31 positions, or targets, for materials to be irradiated. A total of seven targets were used in the work on element 117.

This is the second discovery of a new element for ORNL (61 and 117). Oak Ridge isotopes have also contributed to the discovery of seven new elements.

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Scientists and Industry Use Neutron Imaging to Improve Energy Efficiency

"We are truly pioneering a new field, and this is a unique time for all of us."

NEUTRON SCIENTISTS ARE PARTNERING WITH INDUSTRY TO ENHANCE ENGINE AND COMMERCIAL cooling technologies in hopes of making improvements that will optimize fuel and energy efficiency.

Hassina Bilheux, a physicist and the lead for developing ORNL's neutron imaging capabilities, uses cold neutrons at HFIR's CG-1D beam line to image automobile engine system components, two-phase fluid components in commercial cooling systems, and electrodes used for lithium batteries.

Neutron imaging is just taking off at ORNL, and although there aren't yet any instruments devoted exclusively to it, Bilheux and her colleagues have been using one of the cold neutron beam lines at HFIR for imaging work. "These are not imaging beam lines," says Bilheux. "But we have been very successful since we started in December 2009 preparing CG-1D for imaging."

Bilheux hopes eventually to bring neutron imaging capabilities to SNS, where she can better and more cost-efficiently select the energy of the neutrons. SNS, she says, has a wide range of energies that makes it possible to image thick samples, which isn't possible at HFIR.

Progress is visible now in a series of industrial research projects already afoot or in the planning stage. Two of the projects under way involve vehicle technologies: producing two- and three-dimensional images of exhaust gas recirculation (EGR) coolers and images of diesel particulate filters (DPFs), which remove the black soot cloud so often associated with diesel exhaust. In both cases, the goal is to improve fuel efficiency and, in the case of the DPF project, to consider the emissions and materials impacts of the introduction of biofuels.

To take measurements, researchers set a sample in the beam and use a detector behind it to collect the neutrons that are transmitted, literally taking shadow pictures of the sample. "Neutrons are especially great for engineering applications because they don't see metals very well but are efficient at seeing hydrogen-rich fluids," Bilheux explains.

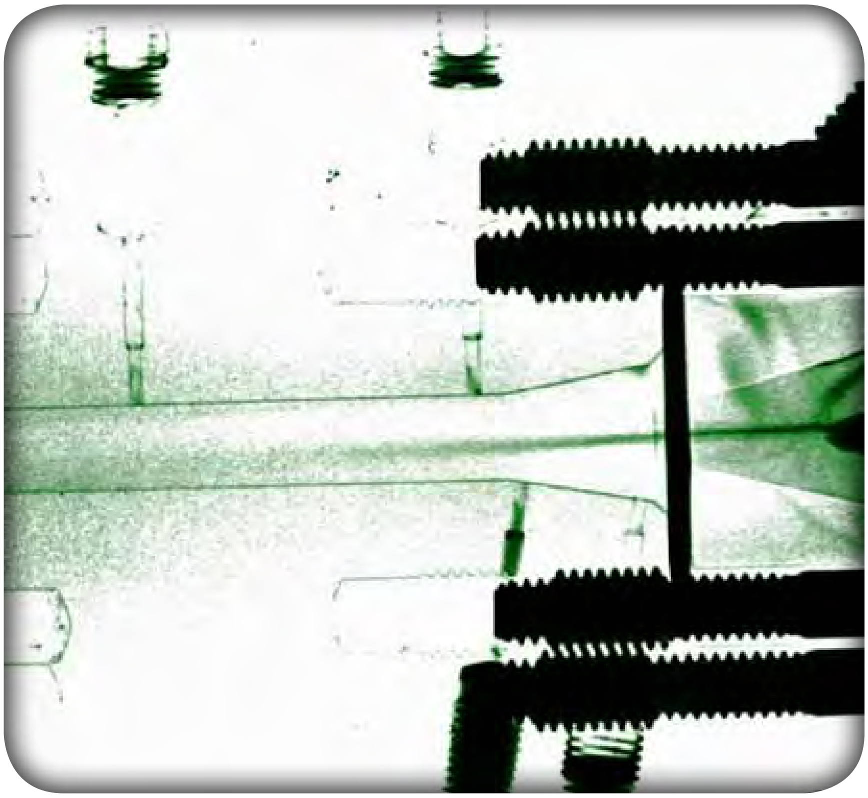
Hassina Bilheux at CG-1D.

In the EGR coolers project, researchers measured coolers from 10 participating companies.

Neutron imaging measures how the hydrocarbon (enriched particulate matter) is deposited within an EGR cooler that shows significant clogging. The role of the coolers is to lower the oxygen content and the combustion temperatures, thereby reducing the formation of NOx (nitrogen oxides) in the cylinder. Thanks to imaging, the researchers can measure the thickness and hydrocarbon content of the deposit and come to understand the spatial and time dynamics of particulate matter deposition. In future measurements, tomography will be used to image complete, intact coolers in three dimensions.

A second vehicle project concerns how soot and ash build up in the DPF of a diesel-powered vehicle and the impact of fuel type. DPFs were developed to remove the particulates (primarily soot) once common in diesel engine exhaust. Bilheux is working with researchers at the Fuels, Engines, and Emissions Research Center (FEERC) at ORNL's National Transportation Research Center. At FEERC, the researchers use diesel engines operated on dynamometer platforms to introduce particulates to the DPF. This enables the study to occur on real engines under industry-relevant conditions; additionally, field-aged samples have been provided to the FEERC researchers from industrial partners.

The work began with measurements of DPFs at different soot and ash loadings. As the neutrons are able to penetrate the ceramic filter, they can take measurements of the hydrocarbon-rich particulates (soot) and metal-oxide–based ash. Although these materials are not necessarily highly sensitive to neutrons, they have a high surface area and are very hydroscopic (readily attracting moisture). The adsorbed water allows detection by neutrons. Neutron tomography is used to view and measure the thickness of the soot in the channels and the location of ash deposits. Ash, mostly from lubricant additives, affects engine efficiency by clogging the filter and increasing the backpressure on the engine and curtails filter life.



Neutron radiograph of a functioning ejector spray.

Bilheux is also engaged with computational scientist Sreekanth Pannala and battery expert Jagjit Nanda at ORNL, as well as industry partners, to measure lithium transport inside complex electrodes.

“This is an important research area for DOE and involves substantial participation by industrial partners,” Bilheux says. Battery storage devices have excellent energy and power-to-weight ratios and are now the power source of choice for cell phones, cameras, and notebook computers. Lithium batteries are also used extensively in biomedical and military applications, and prospects are good for the use of lithium batteries in transportation in the future.

Bilheux is also working on multi-constrained jet flow with the United Technologies Research Center. Neutron imaging is being used to examine jet flow under different conditions to investigate new design capabilities for multiphase ejectors that can improve heating, ventilating, and air-conditioning system efficiency. There are currently no data on internal ejector flow to validate physical models needed to improve ejector design. Neutron imaging can provide these data (see accompanying illustration).

Says Bilheux, “SNS and HFIR, to me are like a train, and it is on a fast pace, and you just jump on it and go with the flow!”

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Neighborly Assistance: VULCAN Lends Unique Capabilities to Diagnosing ITER Cables

Superconducting cables in a fusion reactor can expect a hard life, and the VULCAN Engineering Diffractometer at SNS is helping ensure that they can stand up to the stress.

THE VULCAN INSTRUMENT TEAM IS WORKING WITH THE US ITER PROJECT OFFICE TO RESOLVE ISSUES with a critical component of the experimental fusion energy facility, the central solenoid magnet (CSM). The central solenoid, a joint responsibility of US ITER and Japan, is essentially a large transformer that generates the current to drive and control the plasma in the ITER reactor vessel. VULCAN is being used to examine the superconducting cables that make up the CSM.

ITER is the international project to design and build an experimental fusion reactor. The US project office, hosted by ORNL, resides a few miles down the road from SNS.

ITER staff discovered that the CSM cables were losing their current-carrying capacity over time. They generate a magnetic field of up to 13 T, and with constant magnetic cycling, the superconducting wires inside were found to be degrading. The exact cause of the degradation is unclear, but it is suspected to result from the electromagnetic (Lorentz) force exerted on the wires by the high magnetic field and powerful current. Stymied by the problem, ITER officials asked US ITER to consult with scientists at SNS about using neutron scattering to examine the extent of deformation of the cables.

The samples examined at SNS are sections 1.65 inches in diameter and several inches in length. The cables have a complex structure—superconducting niobium-tin wires intertwined with copper wires, all contained in a stainless steel coating. SNS is well suited for studying the thick cables because it has the most intense neutron beams of any pulsed neutron source in the world, and VULCAN is the ideal instrument because it can handle large industrial-sized specimens as well as small lab samples.

The multiphase material making up the cable is perfect for characterization by a time-of-flight

Xun-Li Wang at VULCAN.

diffractometer such as VULCAN, which maps strains and stresses in materials, notes Xun-Li Wang, a distinguished research staff member and leader for Materials Science and Engineering at SNS and HFIR. Using lattice spacing as an atomic-level strain gauge, VULCAN can map deformation caused by the Lorentz force, and "on a fundamental level, we can also study in detail how the critical current in a superconducting wire responds to applied stress and develop a predictive model for the wires," says Wang.

The VULCAN team anticipates studying a full-size cable specimen (3 m long), which will have undergone extensive cycling under a strong magnetic field at a facility in Switzerland. The work will be conducted in collaboration with scientists at Japan Atomic Energy Agency and Japan's Proton Accelerator Complex. Investigating and resolving the issues is expected to take several months.

VULCAN has also been used to observe charge-discharge cycles in a lithium battery in real time. "We were able to see how lithium ions were being adsorbed onto the graphite structure and resolve it on a time scale," instrument scientist Ke An explains. "You can clearly see what's happening as lithium is transferred from one side of the electrode to another. Once you understand this process, you can tune it."

These experiments are examples of VULCAN's unique capacity to measure material behavior under realistic operating conditions. "VULCAN is a versatile instrument that allows us to quickly set up an experiment like the battery studies," says An.

Among the one-of-a-kind capabilities that VULCAN offers for materials research is single-pulse diffraction, which allows data collection on the time scale of a single 1/60 second pulse of the neutron beam. "This opens up new opportunities to study processes that are happening very rapidly, for example, dynamic measurements to show a material changing under extremes of temperature and applied load," Wang says. The instrument team is developing a pump-probe technique using single-pulse capability that will eventually push time resolution to the microsecond level, he says. "This will provide a unique neutron scattering capability to explore materials behavior in real time and uncharted territory."

Another unique feature is a load frame that can apply tension, compression, and torsion loads simultaneously. Most load frames can apply either tension or compression. Torsional loading is rare, much less multi-axial loading created by applying a tensile or compressive load simultaneously with torsion. "It allows us to test specimens under complex load conditions—real loads are never one-dimensional," An says. "We can also do fatigue tests under cyclic loading conditions up to 30 Hz."

The load frame has four axes that move simultaneously—two for tension and compression and two for torsion. It is 2.7 m long, weighs 670 kg, and can be mounted in either a horizontal or a vertical configuration to allow access to a wide range of grain families with different orientations during an experiment. A new capability is being added, allowing rapid in situ heating under load, says An. VULCAN's load frame repertoire ranges down to paper-size frames for small samples.

The sample table that is the base of the VULCAN experiment chamber is a key to its ability to handle large-scale specimens or sample environments, Wang notes. It can position a specimen or equipment weighing up to two tons and measure with better than 10 μ precision.

VULCAN is well positioned to serve industrial users as well as fundamental materials research, Wang says. Plans are to implement a quick-turnaround mechanism that will allow some types of projects to obtain instrument time in a couple of weeks and have results within a month, he says.

Funding for VULCAN was provided by the Canadian Fund for Innovation through McMaster University.

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Neutron Diffraction Finds Hidden Stresses in Materials Critical for Safety, Energy, and the Environment

Metalsa, EPRI, and John Deere are among the partners in these high-impact studies.

WHETHER IT'S THAT KLUNKY NEW HUMMER YOU BOUGHT FOR A SONG, THAT HONEY OF A BMW sports coupe, farm equipment from John Deere, or a pressurized water nuclear reactor, the materials from which they are made contain hidden stresses that affect safety, longevity, even energy efficiency and the environment.

Camden Hubbard and his Residual Stress User Center at the ORNL High Temperature Materials Laboratory (HTML) use the second-generation Neutron Residual Stress Facility (NRSF-2) at HFIR, along with complementary x-ray diffraction instrumentation, to help industrial partners find out where these stresses are. Their input corrects or validates the companies' computational models so that they ultimately can make better, safer, less costly, and more efficient structural materials.

In another project of importance to the country's 100+ pressurized water reactors (PWRs), the team works with the Electrical Power Research Institute (EPRI) and the Nuclear Regulatory Commission (NRC) to detect stresses in the welds on pipes that conduct coolant water from reactor vessels.

Residual stresses are innate to materials. When industry makes a vehicle, the materials are subjected to heat, shot blasting, or laser blasting, as manufacturers modify them to get improved performance and corrosion resistance. "They're always playing with the process to change the residual stresses to minimize the detrimental stress state and maximize the beneficial," Hubbard explains.

When the metal components in a vehicle are welded together, and the vehicle hits the road for several hundred thousand miles, further stresses occur. Such stresses can be either detrimental—opening up the material and contributing to crack formation—or beneficial, compressive stresses that push the materials closer together, making parts last longer.

Today, manufacturers use computer modeling to try to predict the processes within materials. Working with materials scientists at ORNL, they use NSRF-2 to validate their models. "They want to see if their models are making the right predictions so that they can then use the models with more confidence," Hubbard says.

The actual science entails neutron diffraction, bringing a beam of thermal neutrons to diffract off the sample material. At HFIR, a monochromater selects one energy of neutrons to feed through the beam. "When you know the energy and you can see at what angle the neutrons are scattered, you can measure the interplanar spacing, or d-spacing, of the atoms in the materials," Hubbard explains.

The changes in the material may be 100 parts per million, Hubbard says, so this is one of the more precise measurements done with neutron instruments at ORNL.

Three projects currently running at HFIR involve industrial partnerships with Metalsa S. de R.L. (car and truck chassis frames, suspension mod-

Matt Klug from Dominion Engineering, a subcontractor to EPRI, uses NSRF-2 to study stress distributions in joints welded to PWRs, helping to project crack growth and the probability of failure in the welds.

The Neutron Residual Stress Facility maps hidden stresses that affect the performance of materials.

ules, structural stampings, and truck side rails), EPRI and the NRC (PWRs), and John Deere (farm and forestry equipment).

Metalsa makes 50% of the steel frames for trucks and SUVs in North America. The frame is the unifying base of the vehicle to which everything is attached. As a vehicle travels, there are flexing stresses, and the manufacturer wants to know what effect boring holes in the frame to attach components will have on residual stresses in the material.

The team's results could result in saving expensive raw materials and improving fuel efficiency, saving as much as 200 lb per truck.

The collaboration with EPRI and the NRC concerns ongoing questions about joints that are welded to the country's PWRs. In PWRs, the coolant water exits the reactor vessel, typically a carbonized steel, via a large stainless steel pipe that is welded to the vessel wall with a weld called a "dissimilar metal weld."

In their inspections of PWR plants, EPRI and the NRC have discovered that the weld is one of the places where problems occur. The residual stresses at the joint can either close cracks and keep them from breaking, or open cracks faster. The researchers used neutrons to look for the stress distributions so they can project crack growth and the probability of failure. The project is also examining methods that could be used to reduce the probability of cracking and thus improve safety and the operational life of the reactor.

The third project, with industrial partner John Deere, involves stresses in cast materials. When metal is melted and poured into a die, it cools differently at different locations, which sets up residual stresses in the casting.

"They need to be able to predict these stresses to ultimately predict proper performance of the part. So they bring us several parts with different casting operations to see if their computer models for die casting are giving the right answers," says Hubbard.

"We did neutron residual stress measurements on several of these, and it turns out the data predictions from the models and the measurements that we had were pretty good—as good as I ever expected they could be."

Confident that they have it right, John Deere can look at how to optimize the casting, at what temperature, at what speed to do the cooling, now that the computer simulations have been validated by neutron experiments at HFIR.

"This is a big-impact study," Hubbard says. Castings are heavily used throughout all transportation industries, even in jet planes.

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High-Pressure Studies of Gas Hydrates Show Three-Dimensional "Cages" with Unique Properties

Studies of greenhouse gas clathrates under pressure show how their structures decompose.

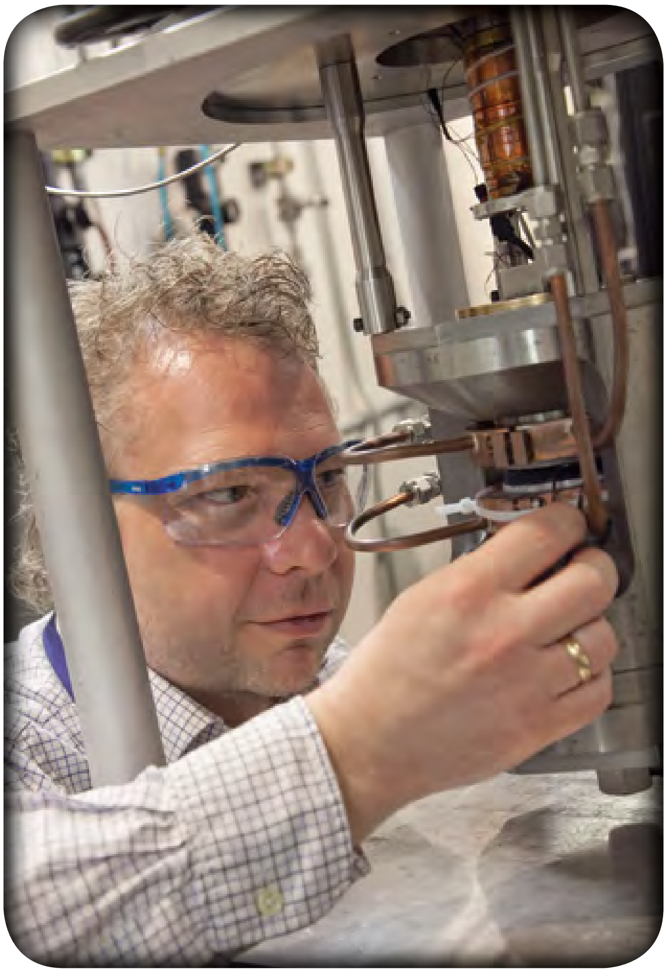
FOR CENTURIES CARBON CONVERTED TO ENERGY HAS BEEN EJECTED INTO THE EARTH'S ATMOsphere as a heat trapping "greenhouse" gas. The most prolific of these anthropogenic greenhouse gases is carbon dioxide (CO_2). It is the challenge of our time to find ways to remove these gases from our atmosphere. One possibility being explored is to react them with water within the Earth, a process that could lead to the formation of clathrate hydrates.

Clathrates are crystalline compounds of water molecules that are hydrogen-bonded to form cages of several types. When stacked together, these cages fill 3-dimensional space. They encage atoms or molecules such as methane, hydrogen, nitrogen, the Noble gases and, most important, CO_2 in an icy crystalline lattice or matrix. Clathrates already exist in nature, some of them tens of thousands of years old, in glacier ice, for example. They also form from methane that escapes through cracks in the ocean floor.

The high-pressure behavior of clathrate hydrates is not now well understood. Researchers want to get atomic-level detail about how they form and decompose. Their decomposition can release large amounts of methane that could affect climate change. But they also have the potential to be used to sequester greenhouse gases and to store hydrogen. Using the SNAP instrument at SNS, scientists have begun experiments aimed at understanding the structural transformation processes in CO_2 and water mixtures.

To make an initial clathrate sample, CO_2 gas at about 100 atmospheres is "balled milled" with ice between 0 and −10°C. At this temperature and under pressure, clathrates form. During the formation process, the water structure that surrounds the methane is disordered. "That has been very difficult to measure because clathrate-forming gases are often very insoluble in liquid water," says Chris Tulk, lead instrument scientist for SNAP, who is engaged with colleagues at the National Research Council of Canada (NRC) and the Carnegie Institution of Washington in this new research.

"If you take pure ice and pressurize it, it changes its structure to other higher-density crystalline forms. If you take clathrate hydrates and do the same thing, they also collapse to high-pressure crystalline forms. However, for CO_2 hydrate, these crystalline forms are largely unknown," Tulk says. The high-pressure capabilities of the SNAP instrument, plus a powerful new array of Anger camera detectors recently installed there, have made it possible to do what Tulk has been dreaming of for years—"Nobody has fully understood the structure of high-pressure CO_2 clathrate before," he says.



Chris Tulk aligns a sample in a Paris-Edinburgh press in preparation for a low-temperature, high-pressure experiment. Tulk and collaborators are engaged in new research on clathrate hydrates.

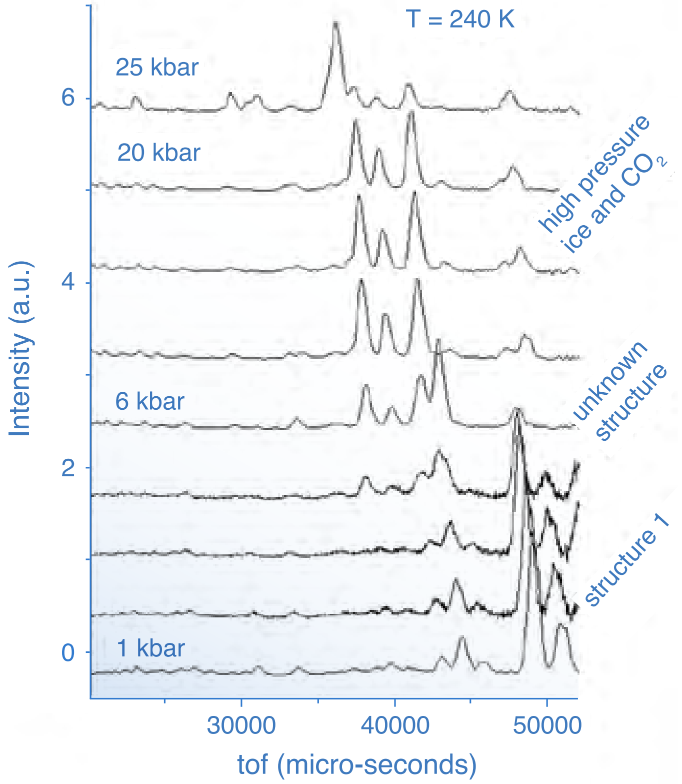
The research team loaded the CO_2 hydrate sample into a press at –196°C, at which the sample is stable at ambient pressure, and connected the pressure cell to the bottom of a cryostat. It was then put on SNAP, pressurized slightly and heated to –30°C, and then further pressurized to around 30 kbar.

Two types of cages are present in the crystal lattice, and under increasing pressure they should collapse. Researchers hope to understand which type is more stable and determine the structure. "Essentially, we want to gain a picture which illustrates the view as if one is sitting on one atom and looking out and seeing where the other atoms are. We sit on the carbon and look at where the nearest waters are or where the nearest carbon is. You get a probability, at a given distance, of finding another atom.

"It became clear that structural transformations begin to take place at very low pressure, near 5-6 kbar. However, the difficulty with this first transformation is that the structure cannot yet be identified. Initial results show that this material is not a traditional, well-understood clathrate structure. However, it does seem that the CO_2 has not been removed from the icy network, meaning that any sequestered CO_2 would remain trapped, though without the structure we cannot predict the relative stability of the material under various conditions," Tulk says (see diffraction plot at right).

Further pressurization resulted in the material decomposing, meaning that the ice and CO_2 phase separated. The result was a pure form of ice known as ice VI and clusters of solid CO_2 commonly known as dry ice. The CO_2 originally encaged in the water was then outside the water network structure. At lower pressures, dry ice decomposes back to gas between −69.5 and −78.5°C. "Further increases in pressure change the ice VI to ice VII, a different crystalline form, but the CO_2 remains unchanged," Tulk says. "And all these transitions occur at relatively low pressures, near and below 10 kbar."

This basic research is likely to be a guide for researchers on the structural processes of CO_2 + water systems. In real-life cases, the mixtures will be "dirty," as they are mixed with other geochemical materials, most notably salts. These will likely change the pressure–temperature conditions of the transformations and could lead to new structures altogether. This will be the topic of follow-on research.



Diffractional plot showing high-pressure transformations in CO_2 clathrates.

In earlier work in 2009 and 2010, the researchers studied xenon clathrates, which form the same type of structure as methane. They found a structure never seen before. Tulk, browsing serendipitously through a chemistry book one day, found a clathrate structure that had been predicted but never found. It looked familiar. He asked postdoc Lin Yang to compare the theoretical model with what they had found in experiment. It was nearly a perfect fit.

"We were excited to find that the structure had actually had been predicted. It was a new structure of gas hydrate that had not been seen before, but we had experimentally produced it."

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Novel Ionic Liquid a Promising Electrolyte for Fuel Cells

Neutron scattering shows diffusion process may boost fuel cell electrolytes.

BECAUSE OF THEIR UNIQUE PROPERTIES, IONIC LIQUIDS COULD HAVE SUBSTANTIAL SCIENTIFIC AND COMmercial importance. Energy-related applications include electrolytes not only in fuel cells but also in batteries and supercapacitors, which rapidly extract current from batteries to operate electric motors.

Sheng Dai, a researcher in ORNL's Chemical Sciences Division, has synthesized a novel ionic liquid form that shows promise as an electrolyte in proton-conducting fuel cells. In collaboration with Eugene Mamontov, chief instrument scientist at the SNS Backscattering Spectrometer, BASIS, and other researchers, he used quasielastic neutron scattering (QENS) to study the diffusion properties of this new liquid.

"A unique property of any ionic liquid is that it does not evaporate because it has no vapor pressure," says Dai. "By contrast, water has a vapor pressure. Thus wet clothes hanging outside in sunlight will dry because water readily evaporates into the warm air." Other useful features of room-temperature ionic liquids, adds Dai, are high conductivity and a large gap between the melting and decomposition temperatures.

When sodium chloride—table salt in solid form—is heated until it melts, the molten salt becomes an ionic liquid, a salt that forms a stable liquid at the salt's melting temperature. It consists of an array of positively charged ions (cations) and negatively charged ions (anions) that move around in the liquid in a process called diffusion.

The new ionic liquid consists of perfluorinated anions and guanidinium cations. The former contain carbon, fluorine, nitrogen, oxygen, and sulfur. The latter are formed by the addition of a proton to each guanidine nucleus, creating a positively charged ion with the chemical power to combine with an anion.

Guanidine is a strongly alkaline crystalline compound containing nitrogen, hydrogen, and carbon [$NHC(NH_2)_2$] that is formed by the oxidation of guanine. It is found in urine as a product of protein metabolism. Guanine is a purine base ($C_5H_5ON_5$) that is an essential constituent of both RNA and DNA.

"Basically what we did was to neutralize strong organic bases using superacids," Dai says.

Dai wanted to analyze diffusion processes in the synthesized salt as both a solid and an ionic liquid. Because neutrons are strongly scattered by hydrogen nuclei, Mamontov and scientist Huimin Luo, also of ORNL, were able to use QENS to distinguish among types of cation diffusion in the liquid.

"We investigated the dynamics of the ORNL-made salt and ionic liquid in detail," Mamontov says. "By using the power of neutron scattering, such as sensitivity to both the time and spatial scale of atomic motions, we got results that cannot be obtained using other techniques, such as nuclear magnetic resonance spectroscopy."

"By using neutron scattering, we got results that cannot be obtained using other techniques," says Mamontov.

Lead instrument scientist Eugene Mamontov (center) and Michaela Zamponi, former instrument scientist, at BASIS.

By adjusting the temperature of the salt, the scientists could study differences in "diffusion jumps" in the novel ionic liquid.

Using QENS, Mamontov's team identified two types of diffusion of cations—long-range translational diffusion and localized diffusion. The faster localized diffusion process is very unusual, but the same ORNL team has confirmed its presence in another novel class of silver complex-based ionic liquids.

"There is a strong possibility that the fast localized diffusion may be common across a wide range of ionic liquids. These two processes, long-range and localized diffusion, occur only in the liquid phase," Mamontov says.

"We can trace the movements of the cations using neutron scattering because they have lots of hydrogen ions," Mamontov adds. "We call the technique 'quasielastic neutron scattering' because the neutrons gain or lose a tiny amount of energy when they collide with protons in rapidly moving cations in the ORNL ionic liquid."

Mamontov, Luo, and Dai concluded that the long-range proton transfer needed for fuel cell electrolytes might be associated with the unrestricted diffusion process in the ORNL ionic liquid. The liquid was recently demonstrated to be a highly efficient electrolyte for fuel cells by the research group of Professor Snyder at Johns Hopkins University (see *Nat. Mater.* **9**, 904 (2010).

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Thermoelectric Materials: Recycling Energy

Ever wonder how a space probe is able to keep going over a long period of time?

FOR SOME YEARS NOW, THE NATIONAL AERONAUTICS AND SPACE ADMINISTRATION (NASA) HAS BEEN using what are called thermoelectric materials to power its space probes. The probes travel such great distances from our sun that solar panels are no longer an efficient source of power. So NASA embeds a nuclear material in a radioisotope thermal generator, where it decays, producing heat energy. That energy is then converted by thermoelectric materials into the electricity that powers the space probe. The same technology is now being explored for more earthly applications, for example, to capture heat lost in the exhaust of automobiles to produce electricity for the vehicle.

Thermoelectric materials are a hot new technology that is now being studied intensively by researchers funded by DOE's Energy Frontier Research Centers (EFRC). Olivier Delaire, a Shull fellow at ORNL, is part of such a collaboration, this one led by an EFRC at the Massachusetts Institute of Technology (MIT). Delaire uses neutron scattering and computer simulation to investigate the microscopic structure and dynamics of thermoelectric materials so that researchers can make them more efficient for new, energy-saving applications.

Thermoelectrics are adaptable for both heating and cooling applications. These materials can convert low-grade heat that is wasted in an industrial process, or in the exhaust system of a vehicle, into electricity. Or they can transport heat from an external source of power and manipulate it to cool a surface.

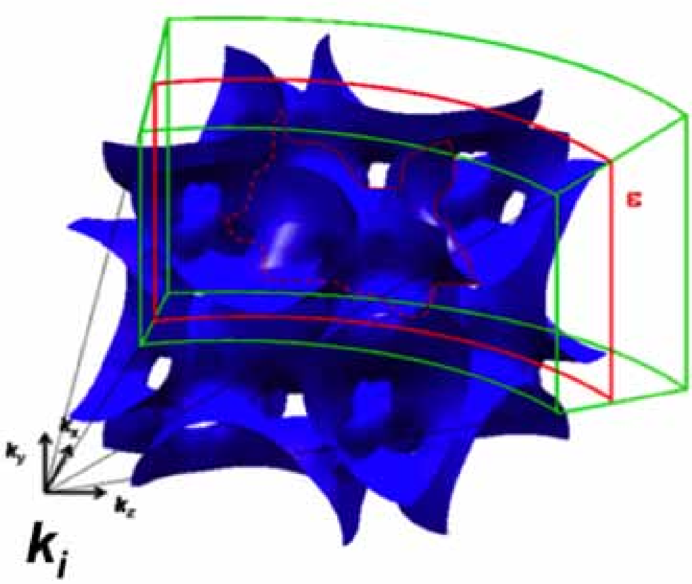
But there are limitations in the materials themselves. "Right now the materials may be on the order of 10% efficiency," says Delaire. "If we can make them two or three times better, if we can get 30% efficiency, that would get people very excited, and it would be much more viable economically."

The research collaboration wants to improve its understanding of phonons, i.e., the atomic vibrations that transport heat through thermoelectric materials. "Neutron scattering is unmatched in its ability to probe the atomic vibrations in the crystals. This is one of the fundamental blocks in the process that we need to understand better."

From left: Olivier Delaire, Steve Nagler, and Todd Sherline.

Here at ORNL, Delaire and his collaborators are using the time-of-flight (TOF) spectrometers at SNS—ARCS and CNCS (the Cold Neutron Chopper Spectrometer)—and the HB-3 Triple-Axis Spectrometer at HFIR. "The SNS instruments offer more power. They can sample the whole parameter space very efficiently. They offer a unique opportunity in a single experiment to sample all the types of atomic vibrations, all the phonons inside the solid. And once we have this information, we can reconstruct the microscopic thermoconductivity, which is really the property we are trying to understand."

The single crystals are grown at ORNL. There are two high-temperature materials, PbTe (lead telluride) and La_3Te_4 (lanthanum telluride) for heat recovery and FeSi (iron silicide) for refrigeration applications. Single crystals offer advantages in neutron science. They can be measured on the TOF instruments at a series of orientations, each orientation giving a comprehensive data



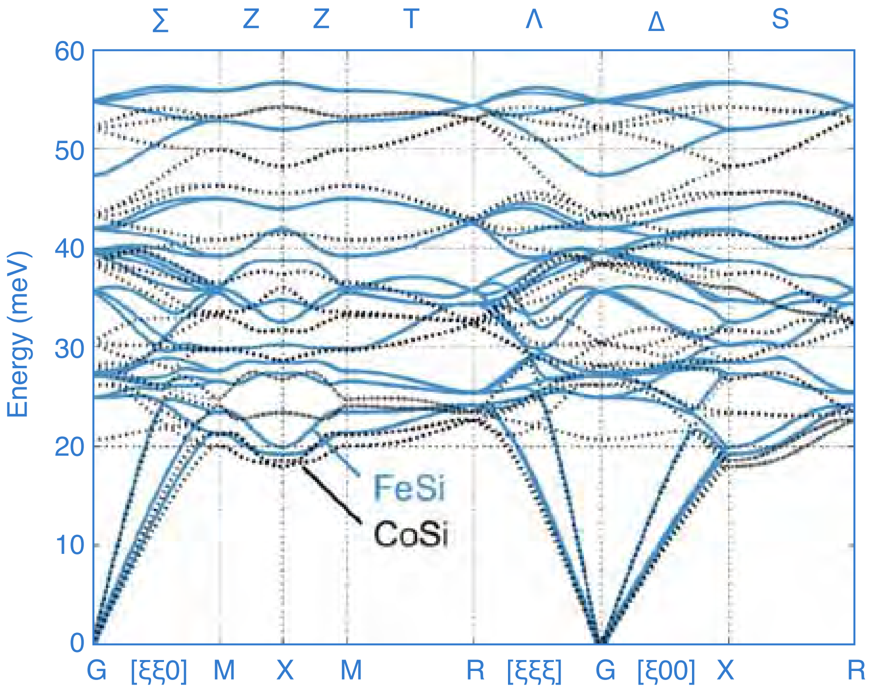
Single-crystal reciprocal space tomography.

set. Combining these sets gives the researchers a complete picture, much like tomography.

“By doing this experiment using the high neutron flux here at SNS we are able to really map out the space, and that is really where the big advance is. Previously we were only able to look at a few points in the space, and that is like looking with a flashlight. With the flux we have at SNS, we turn on the overhead lights and see the whole room all at once.”

Once they have a view of the volume of data, the researchers then use the HB-3 Triple-Axis Spectrometer at HFIR to zero in and look at pinpoints of phonon vibrations in that region. Next, ab initio computational methods simulate the data that the instruments have generated. These simulations are based on quantum mechanics, which gives the researchers a direct comparison between the neutron science measurements and fundamental theory and theoretical predictions.

In 2010, the researchers uncovered an important coupling between thermal disorder and the electronic structure of FeSi. This type of coupling between thermal disorder and electronic structure at finite temperature could prove to be important in many materials, including thermoelectrics.



Calculated phonon dispersion curves for FeSi and CoSi. The calculated dispersion curves for FeSi are in good agreement with the dispersion curves measured using inelastic neutron scattering.

The MIT ERFC team involves a dozen investigators, including Delaire and David Singh, a solid-state theorist in materials science at ORNL. Samples are also contributed by researchers at Boston College. Delaire, Singh, and some of the MIT researchers are involved in the computation.

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Neutron Imaging and Supercomputing Shed Light on a Better Way to Produce Biomass

Integrated research could provide three-dimensional, multiscale information on how component molecules behave at various stages of construction.

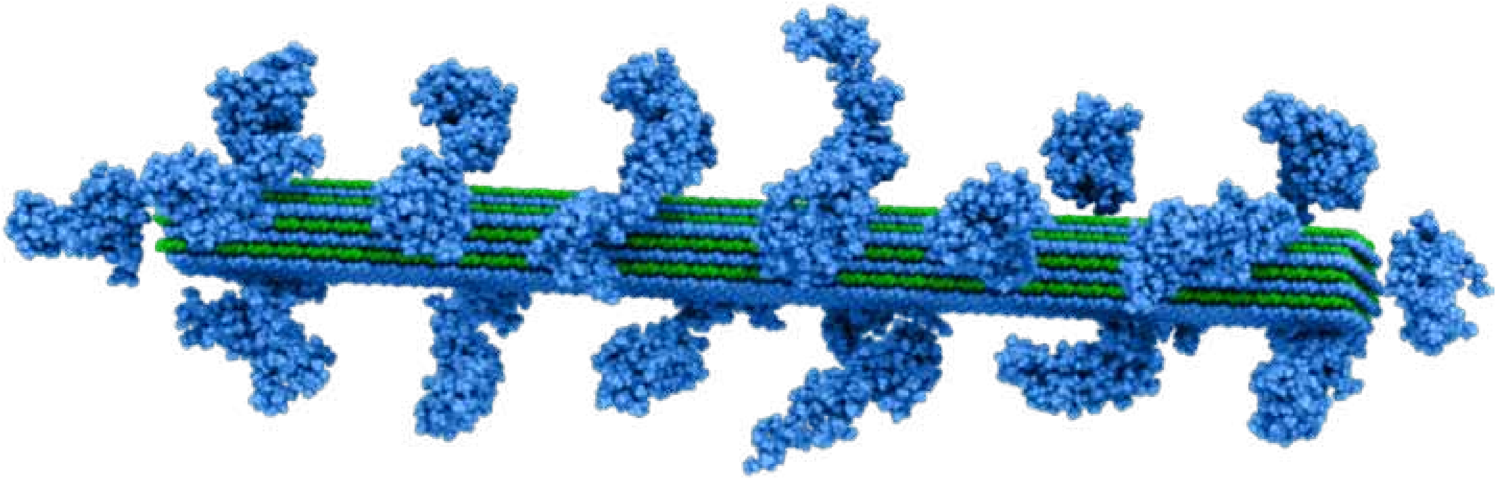
NEUTRON SCIENCE AND SUPERCOMPUTING HAVE TEAMED UP AT ORNL TO PROVIDE NEW, THREE-DIMENsional multiple-scale information on how the component molecules of lignocellulose from switchgrass behave during the stages of pretreatment, breakdown to sugars, and fermentation. In recent results, researchers are observing two key structural changes during biomass conversion: reprecipitation of lignin aggregates and an increase in cellulose crystallite size, consistent with re-annealing the reassociation of cellulose glucan chains into crystalline fibers. These exciting results have recently been published and will directly contribute to understanding and improving biomass pretreatment.

Plant cell walls contain large amounts of cellulose and hemicellulose, polymers of sugars that can be fermented to make ethanol for biofuels. Switchgrass and poplar trees are a more sustainable feedstock than grain from corn. But cost-effective conversion to sugars is hampered by the complex and sturdy laminate structure of the cell walls, the presence of lignin (a polymeric material that forms a protective layer around the wall), and the insoluble crystalline nature of cellulose.

In a multi-institution collaboration, researchers at ORNL are using the Bio-SANS instrument at HFIR and the Jaguar XT5 supercomputer at the Oak Ridge Leadership Computing Facility to visualize and study the pretreatment of lignocellulose with dilute acid. This is a commonly applied industrial process for improving sugar yields from biomass. The process improves the deconstruction efficiency across length scales from the atomic level to the plant's microstructure. A more detailed knowledge of how this is done may enable a targeted improvement in the production of biofuels.

The use of neutron scattering and computer simulation for dynamic visualization of lignocellulose degradation is an integrated, multi-length-scale, real-time imaging program that can visualize biomass structure and its deconstruction during dilute acid pretreatment. Neutron scattering and high-performance computing at ORNL, lignocellulose biochemistry and characterization at the Georgia Institute of Technology, and surface force microscopy at the University of Tennessee are helping to reveal the deconstruction process in unprecedented detail.

Neutron scattering can decipher three-dimensional, real-time information on molecular structures and interactions across a wide range of length scales. To understand the data and build an image of the biomass sample, researchers must also characterize chemical and physical properties



Computer simulation was used to generate a model system of lignocellulosic biomass following dilute acid pretreatment. The model system consists of a crystalline cellulose fiber (green and blue) with clumps of reprecipitated lignin molecules (blue) adhering to the cellulosic surfaces.

Detector tanks for the SANS instruments at HFIR. The Bio-SANS tank is on the right. On the left is the tank for the General-Purpose SANS instrument.

and do the computational simulations and molecular dynamics.

In the next stage of this work, researchers will examine improved varieties of biomass feedstock plants generated by other research groups. Building on the results, they will advance to more complex systems and eventually to the examination of live plant cells during growth and cell wall formation. The breakdown of biomass to sugars by enzymes and microbes will also be examined.

Members of the research team at ORNL are Brian Davison, principal investigator, Jeremy Smith, and Loukas Petridis, Biosciences Division; Barbara Evans, Chemical Sciences Division; Dean Myles, Volker Urban, William Heller, Hugh O'Neill, and Sai Venkatesh Pingali, Neutron Scattering Science Division; and Ida Lee, Department of Electrical and Computer Engineering, University of Tennessee, Knoxville. Art Ragauskas and Marcus Foston are carrying out the preparation and chemical characterization at the School of Chemistry and Biochemistry, Georgia Institute of Technology.

The DOE Bioenergy Research Centers, including the Bioenergy Science Center at ORNL, will characterize and compare biomass samples using this imaging technology. This will expand the power of neutron analysis and simulation into complex soft materials and show its relevance in biology and in renewable energy production technology.

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A New Home for Greenhouse Gases

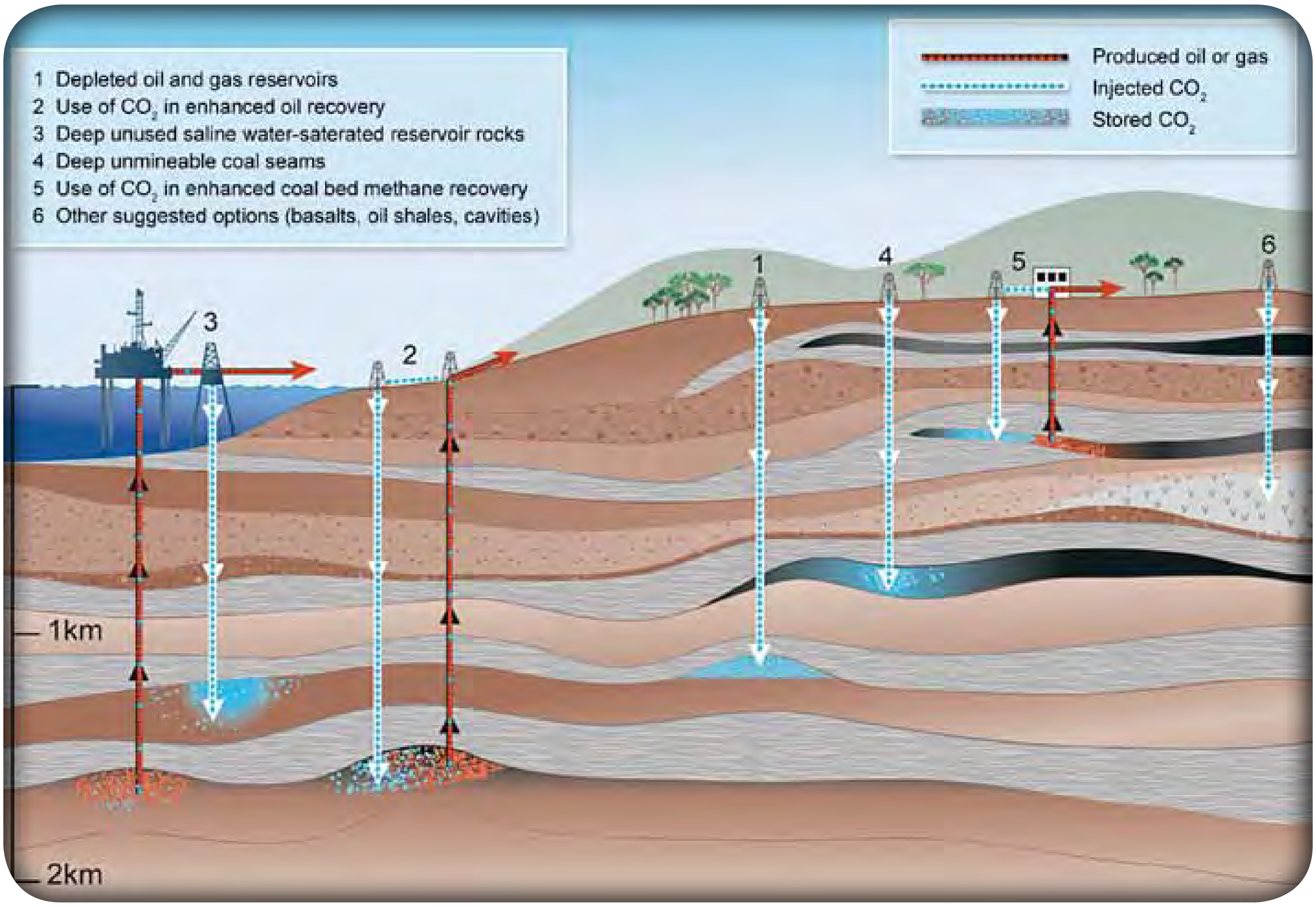
Small-angle and quasielastic neutron scattering map pores for future CO_2 capture and storage.

ONE PROPOSAL FOR ARRESTING THE RISING CONCENTRATION OF ATMOSPHERIC CO_2 IS CARBON CAPture and sequestration in underground natural porous media (saline aquifers, depleted oil and gas reservoirs, and unmineable coal seams). The amount of CO_2 that can be adsorbed by a coal or other porous material is one of the critical parameters for sequestration technology. However, no existing experimental method is yet competent to help researchers understand and predict fluid adsorption capacities in various coals.

For this purpose, researchers led by Yuri Melnichenko of ORNL have used SANS, ultrasmall-angle neutron scattering (USANS), and QENS to assess quantitative, pore-size-specific information on the sorption and mobility of CO_2 into the microstructure of various coal types. The group has developed unique high-pressure cells so that neutron scattering can register scattering patterns over a wide range of scattering angles, at temperature and pressure that correspond to underground conditions in coal seams with a depth down to 10 km below sea level.

The team also developed a novel way to interpret SANS and USANS data that allows them to “look inside” pores and to obtain pore-size-specific information about how well the micro-, meso-, and macropores of coal adsorb CO_2. (1) The advantage over traditional sorption measurements is that small-angle scattering can distinguish the contribution of different pore sizes to the total adsorption phenomenon. The method can be used to study the fluid behavior in any natural or engineered porous system with polymeric, carbon, or inorganic membranes.

SANS and USANS experiments using the methodology developed by the team have revealed unexpected results, such as strong densification of CO_2 in micro- and mesopores of coal (up to a factor of five), which could not be predicted from exist-



Geological storage options for CO_2.

ing models. At the same time, QENS experiments done on BASIS at SNS reveal a dramatic decrease of methane diffusivity in small pores (more than two orders of magnitude), compared with bulk coal (2). Such results demonstrate that small pores work as a “molecular pump” that condenses confined greenhouse gases into liquid.

Accurate interpretation of the scattering from CO_2-saturated rocks requires parallel studies of fluid adsorption in model systems such as porous fractal silica, with known composition and controllable structure. In another 2010 study, researchers used the SANS instrument to monitor CO_2 in pores of different sizes in porous fractal silica and silica aerogel (3,4). The work furthers understanding of the phase behavior of confined fluids, which is of interest for a variety of technologies, including CO_2 sequestration and enhanced coal bed methane (ECBM) recovery technologies.

It is a complex task to establish quantitative relationships between the microstructure and matrix chemistry of a porous solid and the accessibility of its pore space to an invading fluid in an arbitrary thermodynamic state. The methodology described here may be used for in situ quantification of coal pores accessible to CO_2 and methane at temperatures and pressures corresponding to subsurface conditions. Such experiments help to refine existing methods used for calculating sorption capacity of subsurface gas reservoirs and to improve the models used for evaluating the kinetics of methane production from coal seams. Such work provides essential information for ECBM technologies and geological storage of anthropogenic carbon.

This work was performed at the General-Purpose SANS instrument at HFIR, BASIS at SNS, and the BT-5 Double-Crystal Diffractometer at the National Institute of Standards and Technology (NIST). Some of this research also concerns the Illinois Basin CO_2 Sequestration Regional Partnership activity, funded by DOE. The publication of these results has attracted the widespread attention of the Geology and CO_2 sequestration communities and was highlighted in *Chemical & Engineering News* (5).

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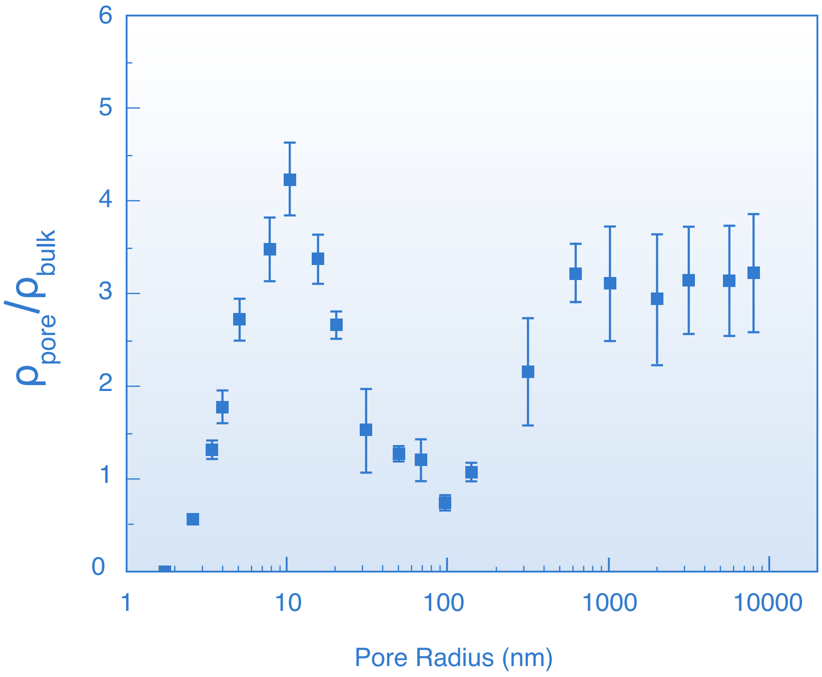

The variation of the ratio of CO_2 density in coal pores and in bulk as a function of pore size.

Neutron Scattering Studies Promise Better Antiviral Drugs

Research into the structural differences of viruses grown in mammal and insects is providing information on how to combat infection in humans.

REARCHERS AT ORNL AND NORTH CAROLINA STATE UNIVERSITY (NCSU) USED THE BIO-SANS INSTRUment at HFIR to do the first ever study of the structural differences between virus particles grown in mammalian and insect cells. Using SANS, they successfully detected and modeled host-specific structural differences. The ultimate goal of this research is to provide critical information on the structural changes associated with infection in order to accelerate the development of antiviral compounds to block the infection process.

Sindbis virus, first isolated in Cairo in 1952, and transmitted by mosquitoes, causes fever, rash, joint pain, and malaise in humans. Sindbis is an arthropod (insect) borne virus or arbovirus. It is maintained in nature by transmission between bird hosts and mosquito vectors. Insect-borne viruses are major threats to health, causing some of the most devastating infectious diseases known to human and veterinary medicine, including Yellow Fever, Dengue Fever, and West Nile Fever.

Collectively, arboviruses are second only to malaria as a threat to global health. About 700 of these agents are currently known, with emerging strains appearing annually. Very few effective vaccines exist. A detailed understanding of the mechanism by which these infectious agents gain entry to cells is essential for the pharmaceutical development of antiviral compounds.

Sindbis is prototypic. Its structure comprises two icosahedral protein shells (i.e., a regular polyhedron of 20 identical equilateral triangular faces, 30 edges, and 12 vertices), separated by a lipid membrane. The inner protein shell—or capsid—protects a core of single-stranded RNA.

Using SANS with contrast variation and modeling, the team was able to detect host-specific

Flora Meilleur prepares buffer samples for measurements on the BIO-SANS instrument.

structural differences. SANS is a structural probe of length scales ranging from 10 to 10,000 Å. It enables the contrast variation method through the unique interaction of neutrons with hydrogen and its isotope deuterium. SANS with contrast variation enables the visualization of components within multi-subunit complexes. When applied to biological complexes in dilute solution, it provides size and shape information that offers insight into function.

Neutron scattering techniques used at BIO-SANS do not decrease the infectivity of the probed virus particles. They show for the first time structural differences between virus particles grown from insect and mammalian cells. The scattering data indicate that, although the radial position of the virus lipid bilayer is not significantly different between the two species, the Sindbis virus grown in mammalian cells has significantly more cholesterol in the lipid bilayer than the same virus grown in insect cells. Additionally, the outer protein coat of the mammalian Sindbis virus was found to be more extended, giving the virus a larger diameter. The SANS data also demonstrate that the mammalian-cell-grown virus has a different distribution of RNA in its core than does the virus from insect cells. The RNA and nucleocapsid protein in the mammalian virus were found to interact closely.

In future work, the researchers will continue to characterize structural changes in these viruses in solution, aiming to discriminate between possible infection mechanisms. Ultimately such work will provide information to accelerate the development of antiviral compounds to block the infection process.

In addition to the BIO-SANS at HFIR, the resources at ORNL's Center for Structural Molecular Biology were used. The collaboration includes ORISE (Oak Ridge Institute for Science and Education) post-doctoral student Lilin He; Amanda Piper, Raquel Hernandez, and Dennis Brown of NCSU; Flora Meilleur, a joint NCSU–ORNL researcher; and Dean Myles and William Heller of ORNL.

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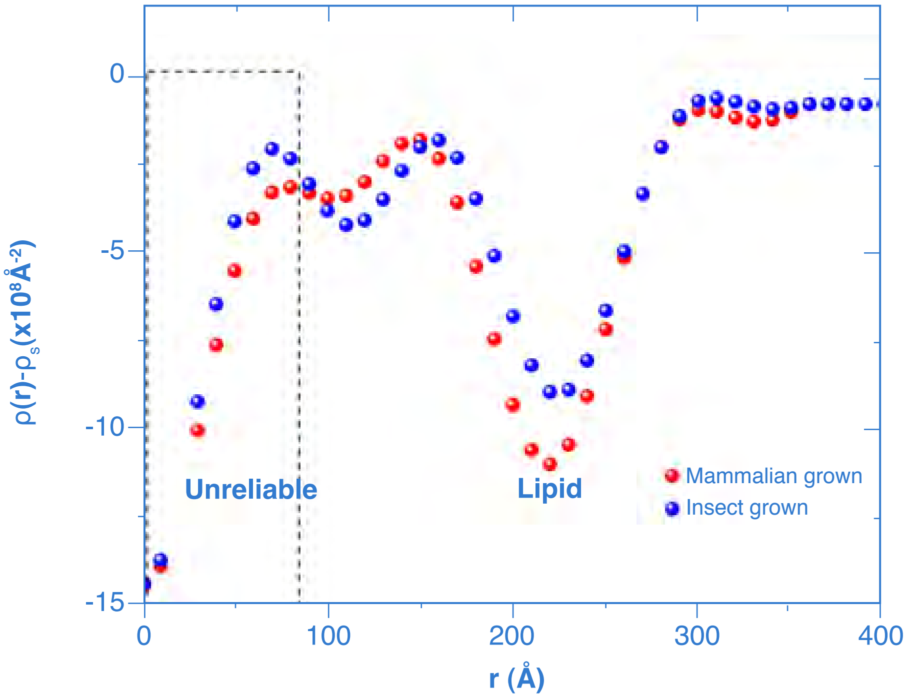

Radial-scattering-length-density distribution function of mammalian-grown and insect-grown Sindbis virus particles. The difference in the depths of the minima is indicative of a difference in composition.

Decoding Magnetic Chatter in Multiferroics

Researchers probe materials that allow magnetic control of electric properties.

RESEARCHERS ARE USING THE COLD NEUTRON CHOPPER SPECTROMETER (CNCS) AT SNS AND THE TRIPLE-AXIS spectrometers at HFIR to study the magnetic dynamics of the multiferroic compound $CuFeO_2$.

Recently, a class of materials called "multiferroics" has been found to exhibit coexisting spontaneous electric polarization and magnetic order. The magnetic ground states of the known multiferroic materials are complex, spiral-like spin structures that contribute to how the material is electrically polarized (ferroelectricity).

ORNL researchers use inelastic neutron scattering (INS) to study how such properties interact at the atomic level. Theoretical modeling and INS measurements clarify the coupling of the electrical polarization with the magnetic order. The research team is Feng Ye, Jaime Fernandez-Baca, Randy Fishman, Jason Haraldsen, Georg Ehlers, and Andrey Podlesnyak.

Using neutron scattering to analyze the elementary excitation spectra of the impurity-doped $CuFeO_2$, Feng Ye and his colleagues can quantify exactly how the magnetic ions are "talking" to the neighboring ions and how impurities in the material affect the strength of the exchange and the resulting spin configuration. They can then design and improve the properties in those materials.

The multiferroic behavior in which the electric properties can be controlled by magnetism occurs in a class of materials known as "frustrated magnets," including rare-earth manganese oxides, delafossite $CuFeO_2$, and other transition metal oxides. Because their electric polarization and magnetic order are strongly coupled, their magnetization can be manipulated with an electric field and their electric polarization with a magnetic field.

"Geometrically frustrated" means that the magnetic ions are arranged in a crystal structure that prevents them from satisfying all their magnetic pair bonds at the same time. Materials do settle into what scientists call a state with a minimal

Andrey Podlesnyak (left) and Feng Ye monitor data collected at CNCS.

energy configuration, but such states may degenerate. Many unconventional and new low-temperature states have been found in these materials in the past decade.

"The current research opens the door to the design of a new class of multifunctional materials with many technological applications, such as novel, high-density, nonvolatile storage and memory devices," Ye says. "This is also an opportunity to demonstrate the power of neutron scattering to understand ferroelectric behavior. ORNL is uniquely positioned to respond rapidly and become the leader in this important field."

Future work with CNCS and the triple-axis spectrometers will characterize the spin dynamics at various concentrations in the impurity-doped $CuFeO_2$. This will allow the team to study the systematic evolution of the magnetism's dynamics.

Ye says that although the magnetic ground state and the low-energy scale produce a complex excitation spectrum, the availability of large computers for simulations, high-quality single crystals for neutron scattering, and the two cold neutron sources will allow them to measure and evaluate the ground state of the magnetic dynamics for the first time.

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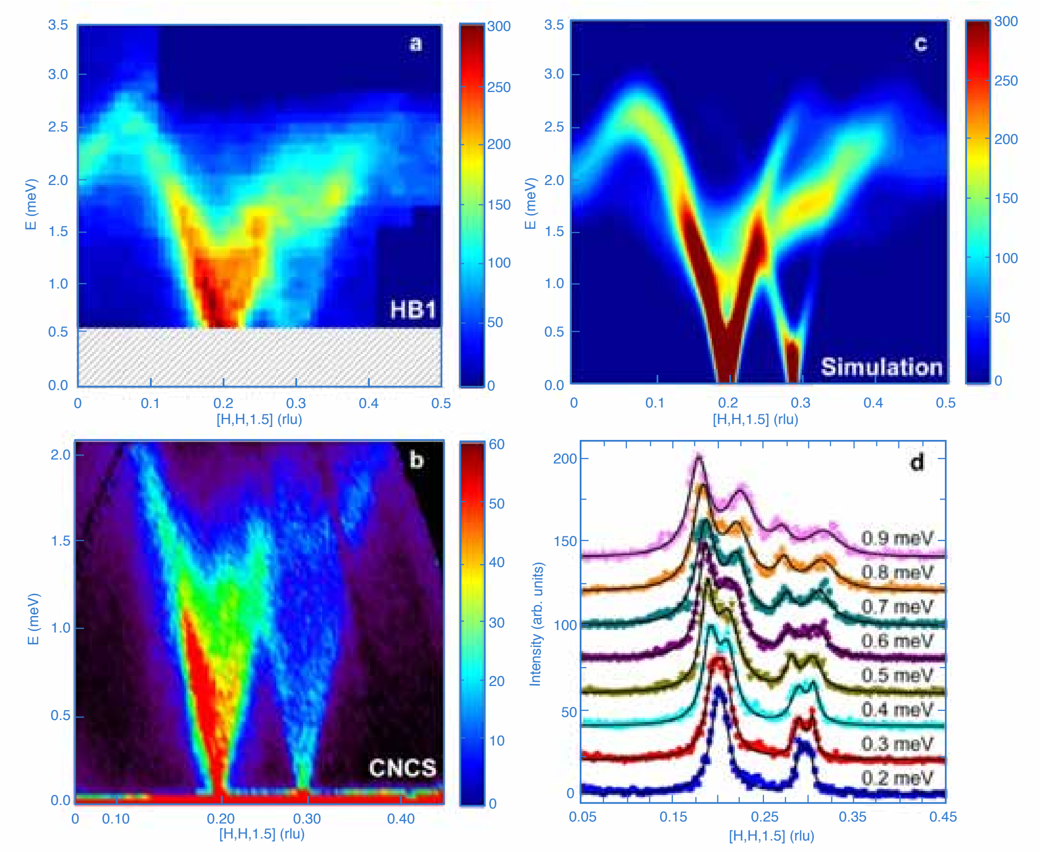

Inelastic neutron scattering spectra of 3.5% Ga-doped $CuFeO_2$ produced by the (a) HB-1 spectrometer at HFIR and (b) CNCS at SNS. (C) shows theoretical simulation and (d) the constant-energy cuts of the SNS data versus momentum transfer.

Biocomposite Material Characterization Benefits Applications in Biotechnology

Researchers from ORNL and the Air Force Research Laboratory investigate the characteristics of a novel composite material with anti-microbial properties.

NEUTRON SCATTERING WAS USED TO STUDY THE PROPERTIES OF A NEW MATERIAL FORMED BY LYSOzyme-templated precipitation of silica, synthesized by sol-gel chemistry. The resilient, functional composite material pairs the protein's microbial properties with silica's structural rigidity.

Mateus Cardoso, Volker Urban, and Hugh O'Neill of ORNL collaborated with Heather Luckarift and Glenn Johnson of the Air Force Research Laboratory on the work. Biomineralization reactions are common in nature, where such composites generate complex architectures that are often superior to those in inorganic materials alone. These biomineralization reactions have become a versatile tool for nanobiotechnology. Understanding how proteins interact with the silica is key to optimizing this process for practical applications.

SANS experiments carried out at HFIR were combined with electron microscopy analysis to understand the assembly and organization of the lysozyme-silica composite material. The material was formed via an in vitro biomineralization reaction. Using SANS with contrast variation, the scattering signatures of the lysozyme and silica within the composite were separated. Contrast-variation methods exploit the unique interaction of neutrons with hydrogen and its isotope deuterium.

The research determined that the lysozyme molecules are spatially correlated in the material and form tightly packed clusters with colloidal silica particles. The size of the clusters determined by SANS agrees well with the structural architecture observed by transmission electron microscopy. Furthermore, scanning electron microscopy showed that the clusters coalesce to form larger quasi-spherical structures (~450 nm) that aggregate to form the macroscopic composite material.

The results indicate that the composite has a hierarchical structure, an important insight into its organization. In addition to demonstrating a well-organized sol-gel synthesis that generates a functional material with anti-microbial applications, the analysis and modeling approaches can be used for characterizing mesoporous and ultra-structural materials.

M. B. Cardoso, H. R. Luckarift, V. S. Urban, H. O'Neill, and G. R Johnson, "Protein localization in silica nanospheres derived via biomimetic mineralization," *Adv. Func. Mater.* **20**(18), 3031 (2010). http://onlinelibrary.wiley.com/doi/10.1002/adfm.201000144/pdf.

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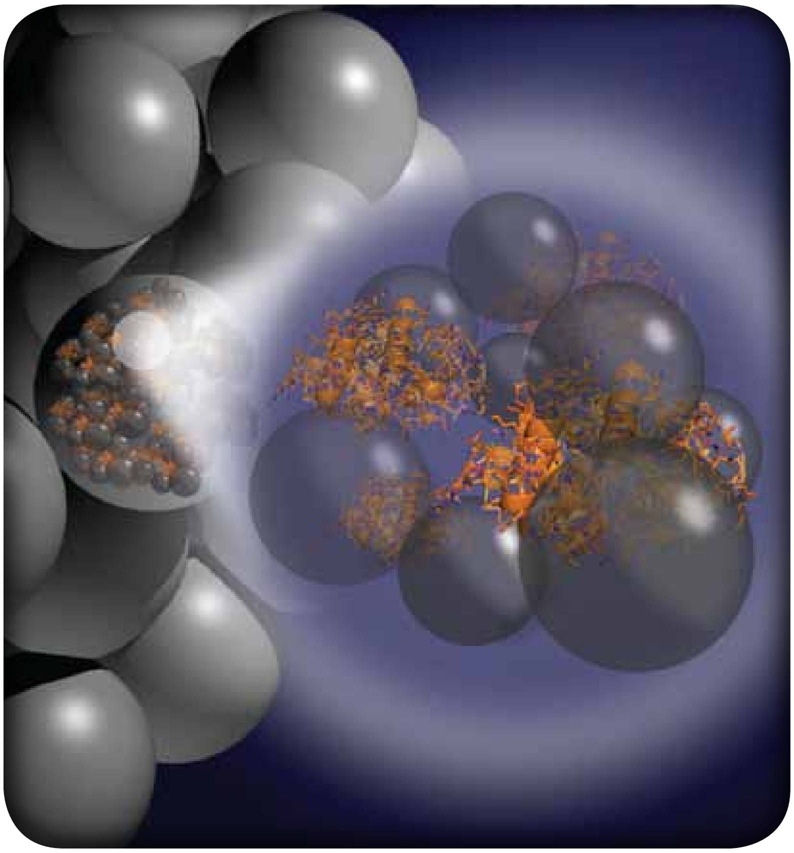


Nanoscale clusters of lysozyme and silica colloids that in turn agglomerate to form microparticles. The biosilica exhibits antimicrobial activity and can also accommodate other proteins or nanomaterials to broaden its functionality.

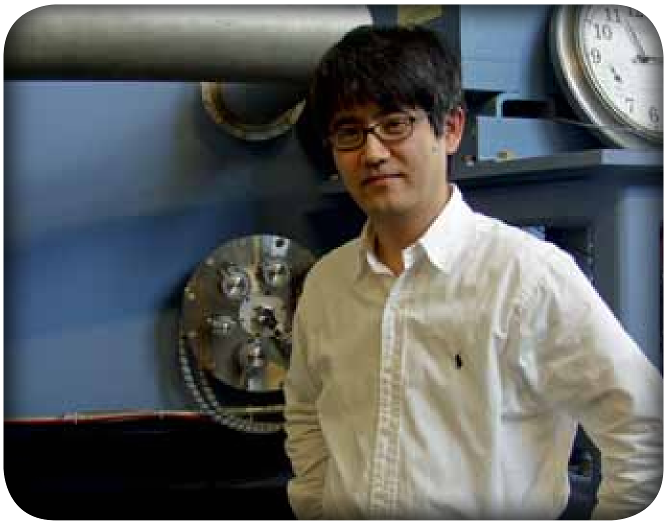
Improved Microscopic Pictures of Polymers

Neutron scattering reveals polyelectrolyte dendrimers can be tailored for biomedical and energy applications.

NEUTRON STUDIES AT HFIR AND SNS FACILITIES HAVE CLARIFIED THE MICROSCOPIC PICTURE OF the structure and dynamics of polyelectrolyte dendrimers, increasing the prospect that these man-made dendrimer polymers can be used in a wide variety of contexts, from biomedicine to sustainable energy.

A SANS study of the structure of polyamidoamine dendrimers (PAMAM) at HFIR has shown that these important macromolecules increase in size and that the intramolecular space is redistributed when they become charged in a D_20 water solution. A second study of the dendrimers' dynamics at the SNS BASIS instrument further shows that when the charge is increased, the local dynamics of a dendrimer's segments are significantly enhanced. These findings provide the critical microscopic picture needed to develop various polyelectrolyte dendrimers to achieve specific targeted functions.

Polyelectrolyte dendrimers are hyper-branched macromolecules that carry amino groups. When PAMAM dendrimers are dissolved in water, the association of the amines and free protons causes the macromolecules to become charged. Despite the surging interest, researchers still do not have a fundamental understanding of the dependence of the structural and dynamical characteristics of polyelectrolyte dendrimers on the molecular charge.



Wei-Ren Chen at BASIS.

The structural study using SANS clearly reveals that as the polyamidoamine dendrimers become more protonated in a D_20 solution, both a gradual increase in the molecular size and a continuous redistribution of the intra-molecular density occurs. This observation is contrary to the current understanding based on computational studies that repeatedly predict that crowding of the atoms will stiffen the local motion of dendrimer segments, hindering exploration of available free volume between the dendrimers and inhibiting electrostatic swelling.

In contrast to the progressively sluggish picture predicted computationally, the dynamical study at BASIS unambiguously shows that upon increasing the molecular charge, a significant enhancement occurs in the local, segmental dynamics of the polyelectrolyte dendrimers.

Researchers at ORNL and several other institutions are using an integrated approach that combines SANS at HFIR, backscattering spectrometry at SNS, theoretical mean-field analysis, high-resolution nuclear magnetic resonance, and isotopically tailored synthesis at the Center for Nanophase Materials Sciences (CNMS) to provide the understanding needed to predict the relation between molecular charge and the properties of polyelectrolyte dendrimers.

The institutions engaged in the research are ORNL, JINS, the NIST Center for Neutron Research, National Tsing Hua University, Taiwan; City University of New York; Rensselaer Polytechnic Institute; Institut Laue-Langevin; and the University of Tennessee.

Y. Liu, C.-Y. Chen, H.-L. Chen, K. Hong, C.-Y. Shew, X. Li, L. Liu, Y. B. Melnichenko, G. S. Smith, K. W. Herwig, L. Porcar, and W.-R. Chen, "Electrostatic swelling and conformational variation observed in high-generation polyelectrolyte dendrimers," J. *Phys. Chem. Lett.* **1**(13), 2020 (2010).

X. Li, M. Zamponi, K. Hong, L. Porcar, C.-Y. Shew, T. Jenkins, L. Liu, G. S. Smith, K. W. Herwig, Y. Liu, and W.-R. Chen. "pH responsiveness of polyelectrolyte dendrimers: A dynamical perspective." *Soft Matter,* **2011**(7), 618, (2011). DOI: 10.1039/C0SM00671H.

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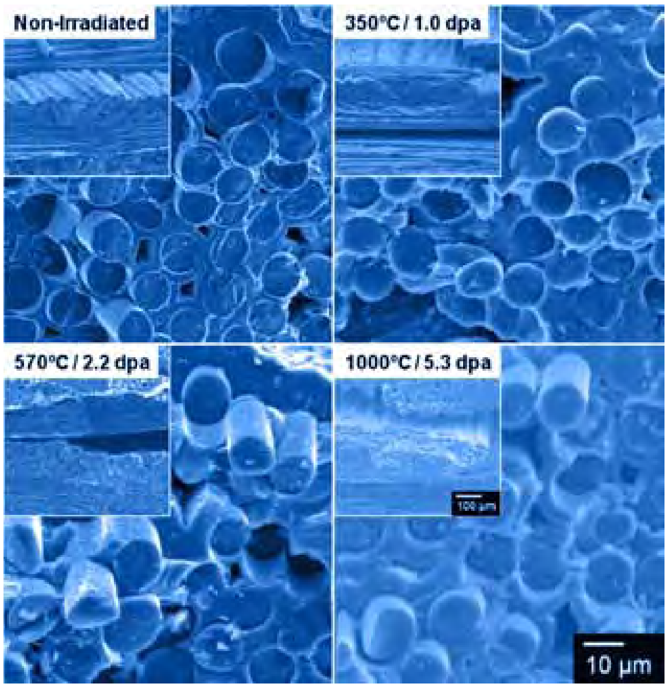
Advanced Materials for Nuclear Applications

Neutron irradiation studies confirm silicon carbide retains pre-irradiation tensile properties.

RESEARCHERS AT HFIR HAVE MADE AN IMPORTANT STEP IN DEVELOPING ENABLING MATERIALS FOR extremely high-temperature nuclear applications in future fusion, gas-cooled thermal, and gas-cooled fast reactors. Their findings confirm for the first time that silicon carbide (SiC) composite ceramics retain their pre-irradiation tensile strength when irradiated at ~910°C.

Radiation-resistant SiC composite ceramics were first developed at ORNL and have become the focus of intense scientific attention. Fiber-reinforced SiC matrix composites are outstanding for their radiation stability, chemical inertness, and reproducibility and quality control. There remain critical unknowns about their reliability during prolonged service in extremely harsh environments, their properties databases, and the design codes for specific applications.

Researchers recently used HFIR and the Advanced Test Reactor in Idaho to successfully record statistically significant results for the thermophysical and mechanical properties of SiC and SiC composites with high-purity, chemically vapor-infiltrated (CVI) SiC matrices that were subjected to the effects of neutron irradiation at elevated temperatures. Five ceramic materials were tested: Hi-Nicalon™ Type-S (HNLS) -reinforced CVI SiC matrix composite, Tyranno™-SA3 (SA3) -reinforced CVI SiC matrix composite, CVD SiC, bare HNLS fiber, and bare SA3 fiber. The materials were subjected to neutron irradiation at up to ~5.3 displacements per atom (dpa), at up to ~1000°C. HNLS and SA3 are the only commercially available SiC fibers the researchers have identified as radiation resistant.



Electron microscopy of fracture surfaces.

Researchers were able to confirm that a statistically significant specimen population of the composite ceramics retains the pre-irradiation strength of their tensile properties at an unprecedented ~910°C. They also found that the thermal conductivity degraded in a distinctly different way among the ceramics tested, regardless of the irradiation conditions.

It was found that neutron irradiation had no significant effect on the tensile properties of the composites, except for an anomaly case of the HNLS composite, which was irradiated in a specific condition. In the single-filament tensile evaluation, both the HNLS and SA3 fibers retained their original strength during irradiation at intermediate temperatures but significantly deteriorated during bare fiber irradiation at ~910°C. Such a deterioration in fiber strength was not observed when the composite material was irradiated.

Composite properties such as strength are determined by three factors: fiber, matrix, and interface. Scientists know that fiber-matrix interfacial friction is the key mechanism underlying the toughness of ceramic composites. The combined results suggest that under high-temperature irradiation, the fiber-matrix interfacial friction of a smooth interface decreases, whereas the friction of a rough interface does not. The researchers consider this important knowledge toward further optimization of SiC composites for high-temperature nuclear applications.

Y. Katoh, L. Snead, T. Nozawa, S. Kondo, and J. Busby, “Thermophysical and mechanical properties of near-stoichiometric fiber CVI SiC/SiC composites after neutron irradiation at elevated temperatures,” *J. Nucl. Mater.* **403**, 48 (2010).

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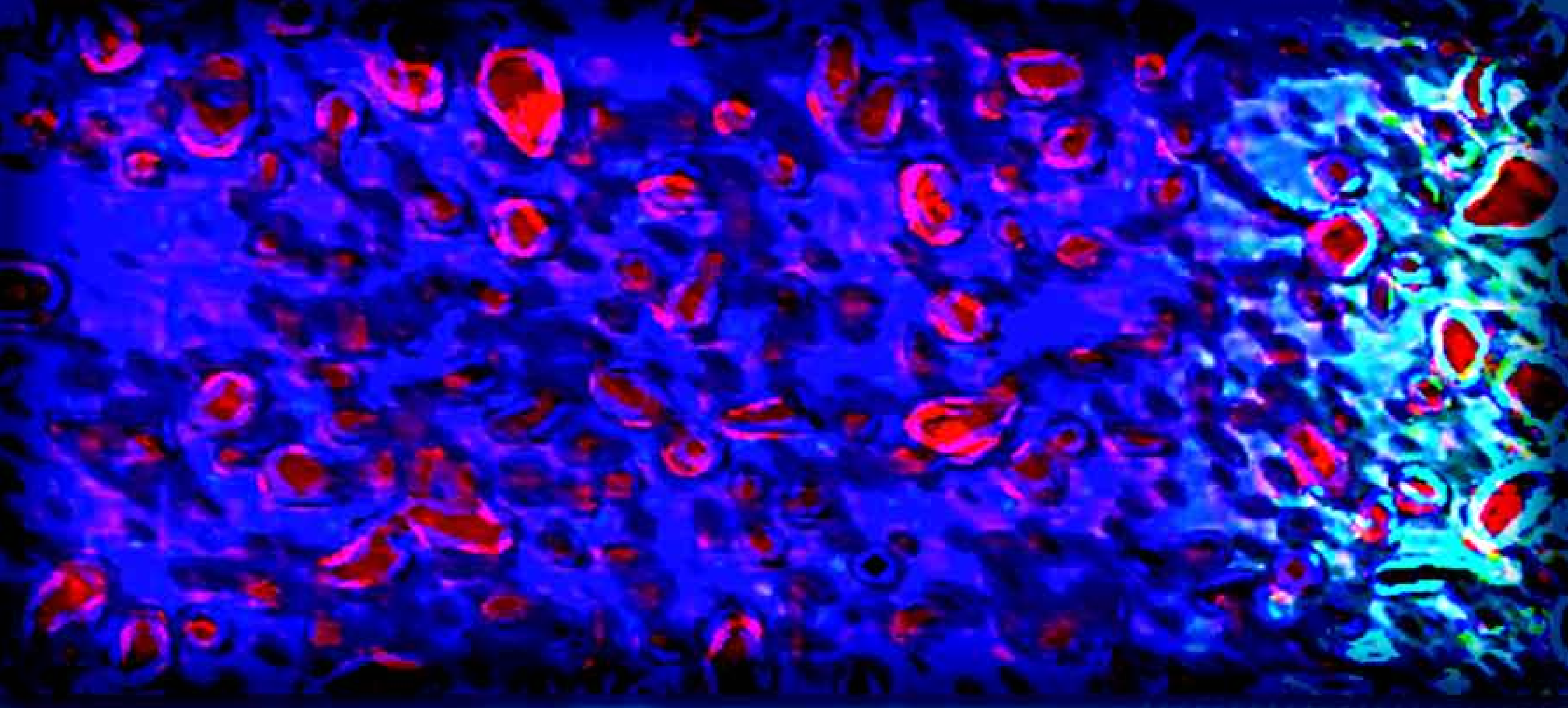


TECHNOLOGY HIGHLIGHTS

Most Powerful Pulsed Source Now One of Most Reliable

Accelerator reliability averaging more than 92%.

IN DECEMBER 2010, SNS SET A NEW RECORD WHEN THE ACCELERATOR RAN AT 100% RELIABILITY AT 1 MW. "FOR 24 HOURS, IT DIDN'T go down, not even for a minute," says Neutron Sciences Director Ian Anderson.

SNS has experienced steady improvement in the reliability of the accelerator since operations began more than four years ago, while simultaneously increasing the operational power to 1 MW. That achievement has inspired admiration in the accelerator community around the world, Anderson adds.

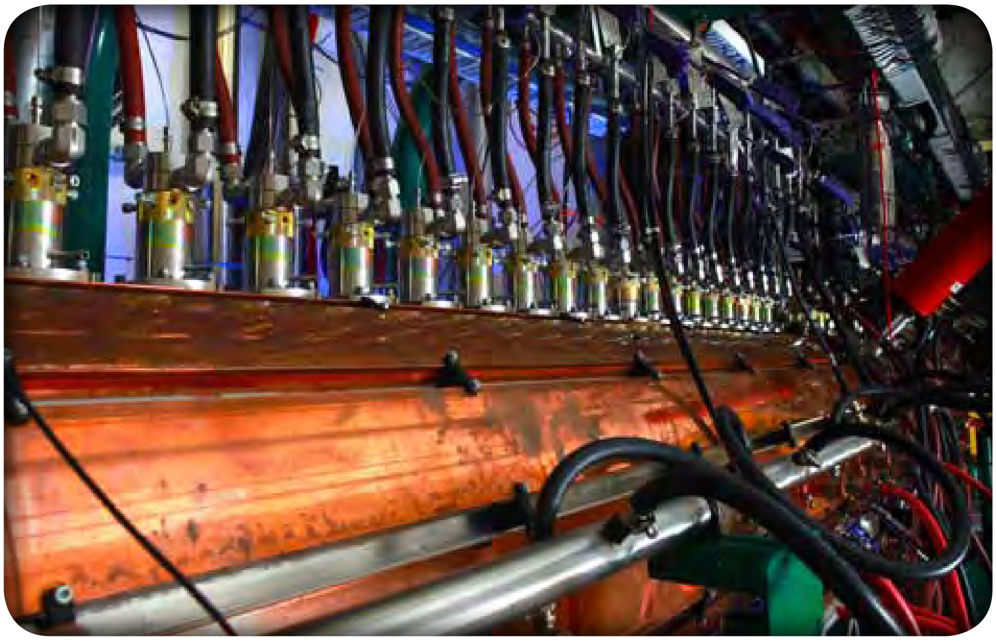
Annual accelerator reliability has climbed from 66% in 2007 to an average of more than 92% to date. "This is a remarkable achievement for such a new accelerator, especially considering it is operating in a pulsed mode at sustained high power (1 MW)," says John Galambos, Accelerator Physics Group leader and technical director of the SNS Power Upgrade Project.

Sustained operation has been achieved with over 98% reliability over a one-week period and with over 95% reliability over a one-month period.

All this adds up to good news for the neutron users. Not only do they have access to the brightest pulsed neutron source in the world, but SNS is also becoming a world leader in the equally important arena of reliability, Galambos says. "High reliability means users can concentrate on their neutron science activities without being bothered by interruptions from accelerator breakdowns."

Accelerator availability is of paramount importance at spallation neutron facilities such as SNS. The accelerator provides the high-power beam that creates the neutrons. No science gets done when the accelerator is down, and because the typical user spends only a few days at a facility, it is vital to keep the accelerator on as much as possible.

High-power accelerators are incredibly complex. They contain hundreds of specially designed electrical, magnetic, and radio-frequency components, all of which must be carefully controlled. The powerful ion beam can destroy accelerator components in less than a ten-thousandth of a second. Sophisticated protection systems must be constantly vigilant, monitoring signals from the equipment and instruments that indirectly sense the beam. At SNS, the beam is pulsed 60 times a second. Keeping all this equipment running 24 hours a day, 7 days a week is tremendously challenging.



Drift-tube section of the 1,000 foot long accelerator. Composed of three different types of accelerators, two thermal and one superconducting, the SNS accelerator is the first of its kind to generate a pulsed beam.

Galambos says that only after many years of operation and optimizing equipment have high-power spallation source accelerators such as ISIS in the UK, the Paul Scherrer Institute in Switzerland, and the Los Alamos Neutron Science Center at Los Alamos National Laboratory approached an annual reliability average of ~90%.

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Helium-3 Stocks Dwindling, Detector Scientists at ORNL Develop Alternatives

Wavelength-shifting fibers and Anger cameras are meeting the need.

THE NEUTRON SCIENCES DETECTOR GROUP, ALONG WITH THEIR COUNTERPARTS WORLDWIDE, ARE WORKing furiously to develop neutron detector technologies that don't depend on helium-3 (^{3}He).

Helium-3 has been the gas of choice for gasous detectors since the early days of neutron science. The demand for it to detect neutrons and measure the scatter off a researcher's sample is steadily increasing. Since 2001, ^{3}He has also been in high demand for Homeland Security portal monitoring.

Bad news. ^{3}He is not found in nature. It is a by-product of the decay of tritium in nuclear reactors, a critical component in nuclear weapons. As countries have decided to reduce the weapons stockpile, the production of tritium has stopped.

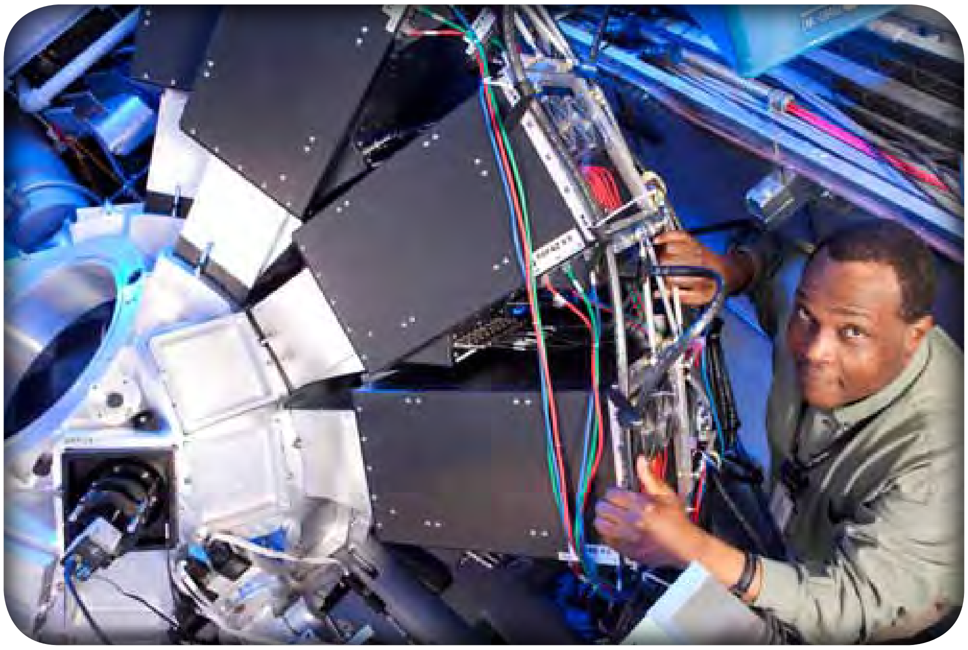
About two years ago, detector scientists worldwide faced the reality that stockpiles of ^{3}He are dwindling rapidly, while demand for it has risen by a factor of five. ORNL is not in immediate trouble, however. SNS and HFIR use four detector types: multi-wire proportional chambers and linear position-sensitive detectors, both ^{3}He-based technologies, and two newer scintillator-based detector systems developed at ORNL that use lithium (^{6}Li).

An international collaboration has begun the search for alternative detector sources. At ORNL, the detector scientists have developed an Anger camera, named for its inventor, and a wavelength shifting fiber neutron detector, in which a large-area scintillator is coupled to an array of photomultiplier tubes by fiber optics.

The ORNL team installed Anger camera arrays at the SNS SNAP and TOPAZ instruments. Says Ron Cooper, chief detector scientist at SNS and HFIR, "the TOPAZ array is completely unique. We got to 900 μm resolution, which had never been done with a mass-produced detector system. We have 10 times as many Anger cameras here as at any other facility around the world. They are also much better: higher-rate capability and higher resolution."

Cooper says the team will be expanding the new technologies to other beam lines, where feasible. "We go after the best detector for the application. So the first thing you do to decide what detector to use is to look at the instrument, look at the science, and then decide what the requirements are for the detector. Then you go after the best solution."

Contact: Diawara Yacouba, diawaray@ornl.gov



Diawara Yacouba, Neutron Facilities Development Division, next to the Anger camera array for TOPAZ. The cameras (rectangular black boxes) are arranged in a sphere around the instrument's sample chamber.

Exciting New Tools for Data Acquisition and Analysis

Remote apps keep users plugged in to ORNL resources.

EXPERIMENTERS AT THE SNS AND HFIR INSTRUMENTS ARE SHADOWED BY A LARGER NUMBER OF USERS taking advantage of remote access systems to view and manipulate data produced by earlier experiments. The Neutron Sciences Data Portal and remote login systems were hosting as many as 130 users a day and 71,000 computing jobs a month by the end of 2010.

“Between run cycles, these numbers give a feel for the activity occurring independent of the beam, work that’s computing related rather than instrument related,” says Steve Miller, who manages the portal and leads the Scientific Data Management Group. “The portal is the Web front end to computing resources users can use remotely to analyze and manipulate their data.”

Web-based systems also provide data translation and job monitoring tools that allow users to check the progress of experiment data creation and data reduction jobs, allowing them to keep tabs on an experiment without being at the instrument.

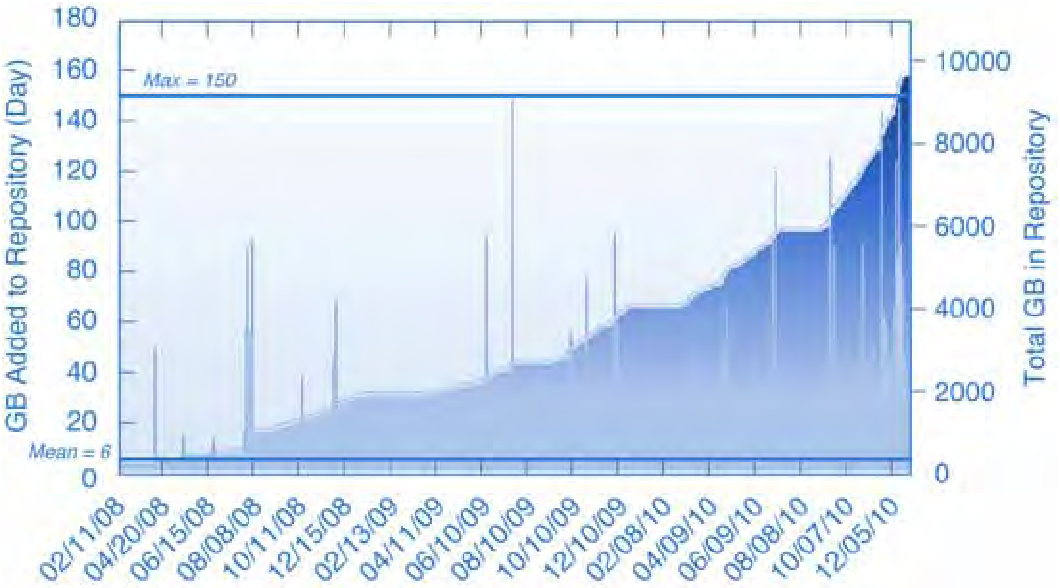
The portal and remote applications give users 24/7/365 remote access to experiment data files, data analysis and management software, and ORNL computing, Miller says. “We’re seeing considerable growth for users running remote applications on our computing resources. By the end of 2010, there were more than 700 different users with computing accounts.”

A class of the Neutron Sciences analysis computers has 32 computing cores and 256 GB of RAM, Miller points out, whereas a typical laptop has 2 to 4 GB of RAM and 2 to 4 cores. Thus users who lack the resources to process their data efficiently otherwise can rely on remote use of on-site computing capacity. Other advantages to working remotely are that users are provided the most recent versions of applications, and they can use the facility to organize and manage their data for them. Shared areas within the experiment data areas also facilitate collaborations similar to storing data “in the cloud.” Data are kept private to the experiment team.

ORNL’s premier storage system could be tapped for data storage.

DATA FILES FOR SNS AND HFIR INSTRUMENTS RESIDE ON A HIGH-CAPACITY, HIGH-PERFORMANCE storage area network. But the need for storage is overtaking the available space. So as a part of planning for user needs, Neutron Sciences is negotiating to use ORNL’s High-Performance Storage System (HPSS), maintained by the National Center for Computational Sciences. The HPSS can store petabytes of data.

Experiment data produced by instruments, plus shared data produced by users, totaled almost 30 TB at the end of 2010, says Steve Miller. That’s up from less than 7 TB in 2009. Shared areas that experimenters use for data



Data produced from experiments and data analysis grew from less than 7 TB in 2009 to almost 30 TB in 2010.

Steve Miller (left) and server administrator John Quigley in the storage area network server room.

analysis account for two-thirds of the data stored. “We’re needing more and more resources for users running data sets after they leave,” says Miller.

The single-crystal inelastic scattering instruments—ARCS, SEQUOIA, CNCS—tend to produce enormous data sets, Miller notes, because they rotate a sample through 360 degrees, taking measurements at every degree or two. “One experiment can be 100 runs or more. Multiply these 100 measurements by the number of pixels per instrument—those get to be very large data sets.”

If HPSS can be used, the plan is to push a daily data archive to the system of tape silos housed on ORNL’s main campus. Users could request data using the portal and be notified automatically when they are available. The whole process should take less than half an hour.

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Mantid—Event mode data reduction and analysis capabilities speed up data for users.

THE MANTID PROGRAM IS AN EXTENSIBLE, OPEN-SOURCE SOFTWARE FRAMEWORK FOR NEUTRON scattering data reduction and analysis built to professional standards of software development. The framework is being developed as part of a collaborative project between the Neutron Sciences Scientific Data Analysis Group and the ISIS Pulsed Neutron and Muon Source at Rutherford Appleton Laboratory in the UK.

Mantid is available for users to download and install on their own computers and can be run on Windows, Mac OS X, or Linux. It efficiently handles large data sets such as those produced by the new generation of neutron scattering instruments at SNS and ISIS. The latest release of Mantid is undergoing robustness testing and will be developed during the next year for all the SNS and HFIR instruments.

Stuart Campbell, lead for the inelastic instrument software team, points out that the work is more than just replicating previous data reduction methods. Because instruments record data in an “event-based” format (see related article on p. 56), “log files” of sample environment parameters can be recorded simultaneously on the same time scale and correlated with the neutron events using Mantid.

Mantid is the first data reduction package to incorporate these event mode methods, Campbell says, and provides a “big step in functionality” that provides greater flexibility for users to explore their data. Combining event mode with the intrinsic multi-threading (parallel processing) capabilities built into Mantid cuts the time required to reduce datasets by more than an order of magnitude.

Apart from event mode methods, Mantid is being developed to incorporate advanced n-dimensional visualization techniques using other open source packages. “If we can take advantage of the parallelization and scalability in those packages, we will enable the users to much more rapidly extract the information they need from their large n-dimensional datasets,” says Campbell.

For more information, see www.mantidproject.org.

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Target Performance Exceeds All Expectations

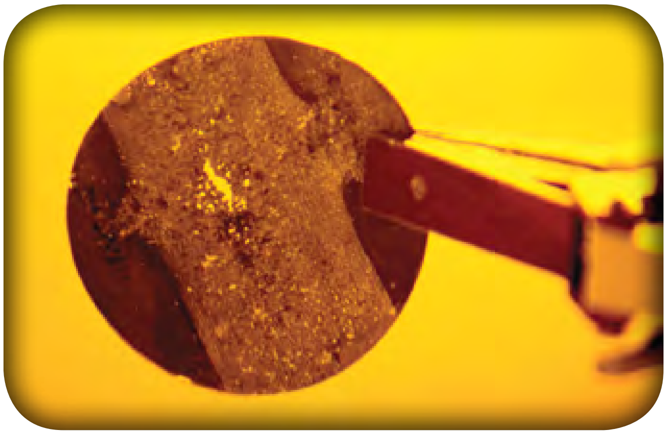
"Can withstand powers in the range of 1 MW for half a year."

DURING THE SUMMER 2010 SHUTDOWN, ONLY THE SECOND MERCURY TARGET INSTALLED AT SNS since its startup in 2006 was replaced. The target had endured a full year of operation with more than 1250 hours of proton beam operation above 900 kW.

This performance exceeded all expectations. "The operational conditions experienced by this target correspond to a radiation damage level that is 50% beyond the lifetime goal that we had originally planned for targets," says John Haines, director of the Neutron Facilities Development Division.

The energetic protons coming from the SNS accelerator do permanent damage to the target casing. As the power of the proton beam increases, the proton bunches coming out of the accelerator smash into the target with such violence that the mercury rapidly heats, locally producing 200 to 300 atmospheres of pressure. The resulting pressure waves hit the vessel surface, bounce back, and form bubbles. As the bubbles collapse, microjets at up to 150 m/s strike the vessel surface and cause pitting and erosion that eventually could penetrate the target walls.

"We have established that the target can withstand powers in the range of 1 MW for half a year's worth of operation," Haines says. "We are quite pleased with this outcome, which confirms the 'wisdom' (some might say luck) of deciding to go with a mercury target."



Cavitation damage on inner wall of first target.

SNS installed and successfully commissioned a new target imaging system in 2009 that helps monitor beam conditions at the target. The imaging system is capable of snapping pictures of the individual pulses as the 1 MW proton beam strikes the mercury target 60 times per second. The new "camera" allows accelerator and target control room staff to monitor and then redistribute the proton beam profile that could otherwise cause structural damage to the target vessel.

The imaging system is starting to pay its way. During some of the initial runs, the team noticed that the beam was peaking more than it should have been. It emerged that an accelerator instrument wasn't working properly. The instrument was corrected and the beam intensity redistributed, with no beam time lost.

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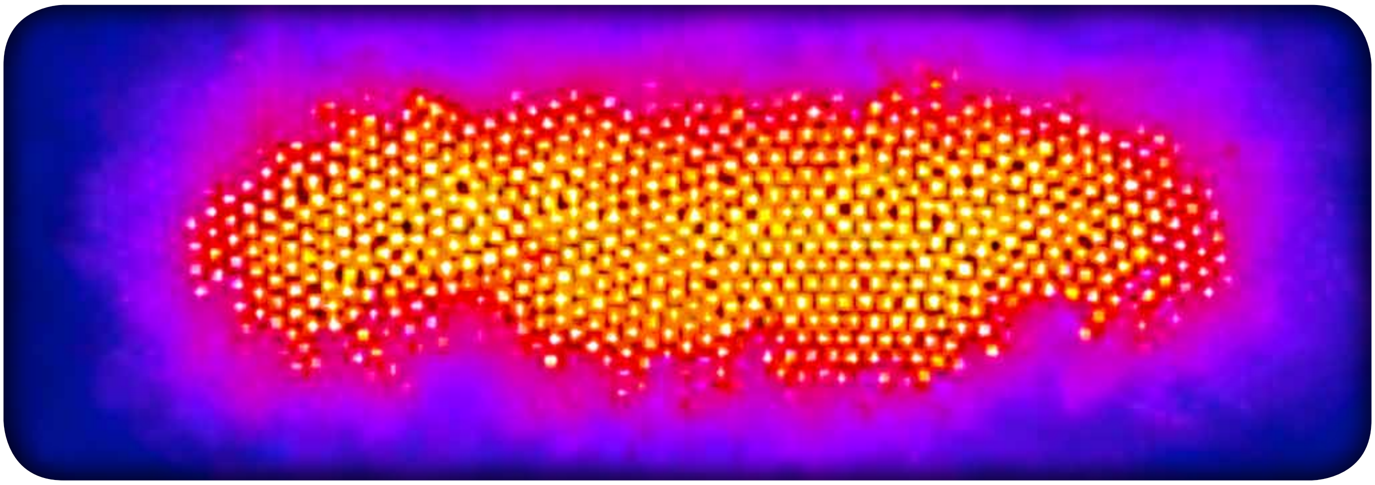

New imaging technology provides a unique view of the SNS target.

New Sample Environments Enable World-Class Science

Hot, cold, magnetic environments continue to expand.

ADVANCED INSTRUMENTS AND POWERFUL NEUTRON SOURCES AREN'T THE ONLY RESOURCES ENABLING great science at SNS and HFIR. The experimental work also depends on having the appropriate sample environments for studying materials under controlled conditions.

One of the hottest, literally, new sample environments now on line at SNS is an aerodynamic levitator, which allows samples to be suspended on a jet of gas instead of placed in a sample can. "Levitation allows us to heat samples to a molten state—temperatures at which a sample can would react with the material inside," says Sample Environment Group Leader Lou Santodonato.

At the other end of the spectrum, a dilution refrigerator (dil fridge) for ultra-low-temperatures was commissioned in 2010 at SNS and used in an experiment in which it reached 50 mK. The dil fridge can be combined with a special cell for studying helium in liquid and solid states—an important new capability for SNS, Santodonato says.

Both SNS and HFIR are building complete collections of magnetic environments. At HFIR, a newly upgraded 4.5 T horizontal field magnet is available, and an 8 T vertical-field magnet is being fabricated. "It will boost the magnetic field strengths available for experiments and provide a more modern, reliable workhorse magnet for them," Santodonato says.

At SNS, a 30 T pulsed magnet was commissioned and used to study the magnetic phases of a sample of manganese tungstate, shattering previous field strength limits for white beam neutron diffraction. The pulsed magnet is an electromagnet rather than a permanent magnet; that is, its magnetic field persists only so long as an electric current is flowing through the coil.

Also in use at SNS is a 16 T continuous field shielded magnet called "Fat Sam," one of the strongest in the world for neutron scattering. The 5 T shielded magnet known as "Slim Sam," introduced to the user program in 2008, is in routine use. A 10 T magnet on order will give the facility a complete suite of shielded vertical field magnets by 2012.


John Christianson, Sample Environment Group, works on Fat Sam.

Other new sample environments include:

- An automated multi-sample changer on the SNS Powder Diffractometer that moves individual samples into and out of the beam automatically without having to stop the beam. It can cool to 10 K.
- A ThermoGravimetrical Analysis furnace that monitors how the mass of a sample changes as it is heated.

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Instrument Development

Spallation Neutron Source

BUILD-OUT OF THE SNS INSTRUMENT SUITE HAS CONTINUED AT A RAPID PACE WITH SIX NEW INSTRUMENTS.

EQ-SANS (Extended Q-Range Small-Angle Neutron Scattering Diffractometer). The EQ-SANS is designed for the study of noncrystalline nanomaterials—such as polymers, micelles, proteins, and other large biomolecular structures—in solid, liquid, or gas form. It was designed to have high neutron flux, high wavelength resolution (precision), and wide Q-coverage.

neutrons.ornl.gov/instruments/SNS/EQ-SANS/
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POWGEN (Powder Diffractometer). POWGEN is a versatile general-purpose diffractometer that enables studies of materials that exist as tiny multiple crystals rather than as single crystals. It is especially useful for studies of energy-related materials such as battery components and membranes for fuel cells.

neutrons.ornl.gov/instruments/SNS/POWGEN/
Contact: Jason Hodges, hodgesj@ornl.gov

Left to right: Ashfia Huq (instrument scientist for POWGEN), Jennifer Niedziela (scientific associate for CNCS), and Luke Heroux (scientific associate for POWGEN) monitor operations at POWGEN.

Neutron Spin Echo Spectrometer.

NSE (Neutron Spin Echo Spectrometer). NSE is an ultrahigh resolution spectrometer useful for research in both soft matter (e.g., polymers, gels, and complex fluids) and condensed matter phenomena such as magnetism and ferromagnetism. Optional, easily accessible operation modes such as ferromagentic- and intensity-modulated NSE enable the detailed investigation of magnetic samples and phenomena. NSE is the best of its class with respect to both resolution and dynamic range.

neutrons.ornl.gov/instruments/SNS/NSE/
Contact: Michael Ohl, ohlme@ornl.gov

VULCAN (Engineering Materials Diffractometer). VULCAN is engineered so that it can test large components, such as an engine or part of a steel beam, to test stresses in structures and understand how materials deform under loading. VULCAN can also be used for spatial mapping of chemistry, microstructure, and texture.

To read about some of the recent work at VULCAN, see “Science Highlights,” p. 22.

neutrons.ornl.gov/instruments/SNS/VULCAN/
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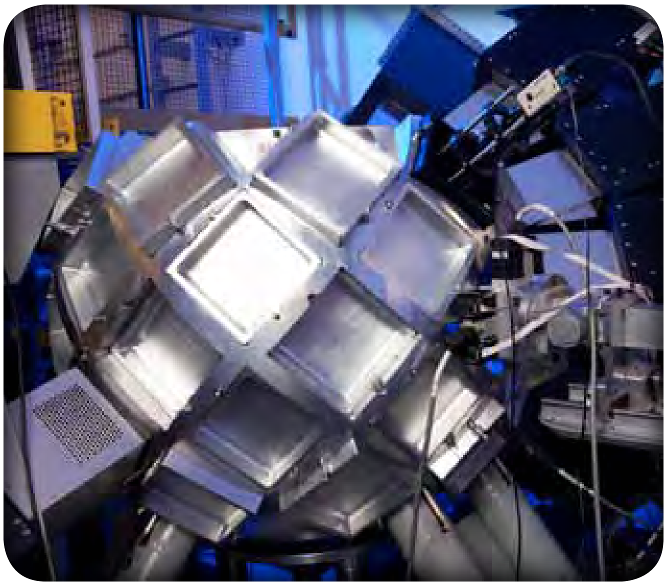

Detector array for TOPAZ.

TOPAZ (Single-Crystal Diffractometer). TOPAZ is designed to probe material structures and responses under controlled conditions. It greatly expands the range of materials that can be explored in chemistry, earth sciences, materials, solid-state physics, and biology and will assist in studies of medical compounds.

Neutron single-crystal diffraction is uniquely positioned to decipher the pathways and bonding of hydrogen in the presence of heavy metal ions, as it is sensitive to both classes of elements in comparable quantity. Simultaneously, because neutrons have a magnetic moment, the magnetic ordering and structure of materials can be investigated.

neutrons.ornl.gov/instruments/SNS/TOPAZ/
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NOMAD (Nanoscale-Ordered Materials Diffractometer). NOMAD is designed to carry out structural determinations of local order in crystalline and amorphous materials. NOMAD enables the study of samples ranging from liquids, solutions, glasses, polymers, and nanocrystalline materials to long-range-ordered crystals.

neutrons.ornl.gov/instruments/SNS/NOMAD/
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For information about all the SNS instruments, see neutrons.ornl.gov/instruments/SNS/.

High Flux Isotope Reactor

THE LATEST INSTRUMENT NEWS AT HFIR IS A NEW COLD TRIPLE-AXIS SPECTROMETER (CTAX) AND APproval for a new single-crystal diffractometer, IMAGINE.

CTAX is in commissioning and should be available later in 2011. One of only two of its kind in the United States, it offers better energy and momentum resolution than most other neutron scattering instruments, as well as the flexibility to observe materials under a variety of sample environmental conditions such as high and low temperatures, high pressures, and magnetic and electric fields.

“While the Cold Neutron Chopper Spectrometer at SNS provides snapshots of broad ranges of energy and wave vector space, the CTAX at HFIR allows for a very detailed and focused view of small regions of this space,” says Jaime Fernandez-Baca, leader of the Triple-Axis Instrument Group. “With the information provided by these two types of instruments, we get a more thorough view of the materials being studied, enabling us to design and make novel materials to meet technological challenges.”

New Cold Triple-Axis Spectrometer at HFIR.

The original CTAX instrumentation was developed at Brookhaven National Laboratory by a Japanese team as part of the U.S.-Japan Cooperative

Neutron Scattering program. The DOE Office of Science funded its relocation and modification for use at ORNL.

www.ornl.gov/info/press_releases/get_press_release.cfm?ReleaseNumber=mr20101019-00/
Contact: Jaime Fernandez-Baca, fernandezbja@ornl.gov

MTSU BRINGS IMAGINE TO HFIR

Middle Tennessee State University (MTSU), NCSU, the Hauptman-Woodward Medical Research Institute, and ORNL have received funding from the National Science Foundation for a new single-crystal diffractometer—IMAGINE—that will be located at HFIR.

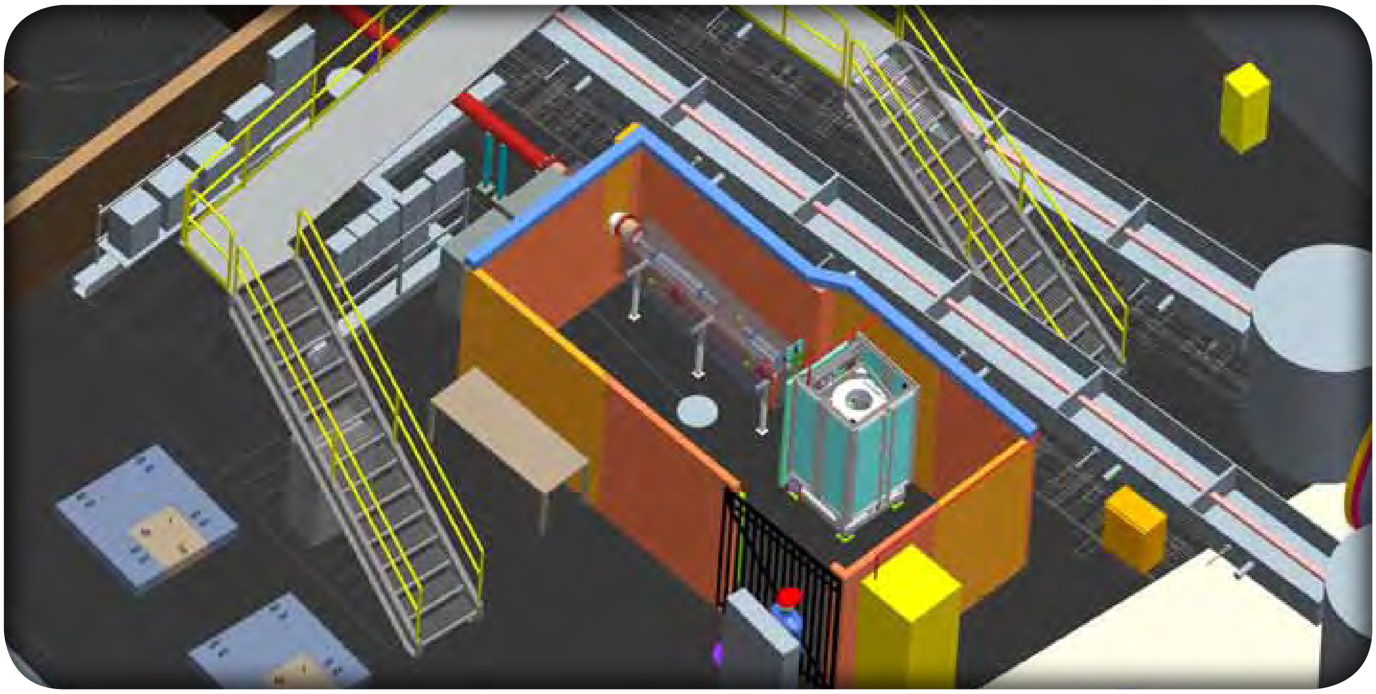
Installation of the diffractometer and neutron optics at HFIR will be complete in 2011. Instrument commissioning will be conducted by principal investigator Tibor S. Koritsanszky, a chemistry professor at MTSU, Flora Meilleur of NCSU, and NSSD's Bryan Chakoumakos, in collaboration with Lee Robertson from the ORNL Neutron Facility Development Division.

IMAGINE will be used to analyze light atom positions in materials of interest across the fields of chemistry; structural biology; pharmacology; condensed-matter physics; nanostructured materials; and the environmental, biomedical, and geological sciences. Beam time will be made available to the national and international user community through the open peer-reviewed proposal system. "This diffractometer will fill a gap in U.S. neutron diffraction capabilities since no similar instrumentation is currently available at a neutron reactor source in the United States," Koritsanszky says.

"Because of HFIR's high intensity of neutrons, we will be able to study the structure of compounds that produce relatively small crystals," Koritsanszky says. "These studies will have an impact in a number of areas ranging from systems of medium-size molecules of biological interest to extended systems containing metal organic frameworks useful in materials research."

neutrons.ornl.gov/instruments/HFIR/imagine/
Contact: Flora Meilleur, meilleurf@ornl.gov

For information about all the HFIR instruments, see neutrons.ornl.gov/instruments/HFIR/.



Schematic of IMAGINE.

USER
PROGRAM

User Community and Services Continue to Grow

From the SHUG Chair

THIS IS AN EXCITING TIME TO SERVE AS CHAIR OF THE SNS-HFIR USER GROUP (SHUG) EXECUTIVE COMmittee (EC). HFIR is operating at full capacity, and SNS has ramped up to an impressive operating power. New beam lines are still under construction, and more instruments enter commissioning and the user program every year, opening up new research opportunities for scientists. This is well reflected in the increased number of proposals, totaling 420 proposals for SNS and 224 for HFIR in the fall 2010 review cycle.

Users also benefit from the availability of other facilities like the Center for Nanophase Materials Sciences, the recently opened Joint Institute for Neutron Sciences, and the new SNS cafeteria. The opening of the new guesthouse at SNS will soon be greeted with much enthusiasm, eliminating lengthy drives to Oak Ridge hotels for users.

The push to advance the availability of instruments and experimental setups at SNS is very aggressive, and we encourage users to voice any concerns that might arise with the SHUG EC. The committee communicates regularly with Neutron Sciences management about user concerns and to help find ways to address them.

A major goal of ORNL management and the SHUG EC is to educate potential users about the benefits of neutron scattering. To this effect, a number of workshops are held throughout the year. These range from specialized topical gatherings to courses for complete novices that are laid out to provide help with instrument selection, experiment design, and proposal writing. A highlight in this respect was the September 2010 workshop on “Neutrons in Catalysis,” which brought neutron and catalysis experts together to explore how neutron experiments could enhance catalysis research.

It is clear that ORNL already offers world-class neutron capabilities, and the spectrum of available resources will only increase over the next few years. Cutting-edge science is conducted at both HFIR and SNS, and we look forward to many more exciting discoveries over the lifetime of these facilities. The SHUG EC is wishing all users stable beams and many exciting results for years to come!

Cora Lind, University of Toledo
cora.lind@utoledo.edu
neutrons.ornl.gov/users/shug

A Growing HFIR and SNS User Community

The Neutron Scattering Science User Program (neutrons.ornl.gov/users) provides integrated support services for HFIR and SNS users. The office assists with outreach and education activities to grow the user community; manages the proposal submission, review, and beam time allocation process; and administers user access, training, and assistance.

The SNS-HFIR user community continues to grow steadily, numbering 1658 total facility users in fiscal year 2010. HFIR and SNS users come primarily from the eastern United States; 56% are from US academic institutions. In 2010, 66% of the users were here for the first time.

The number of proposals received also continues to increase as more instruments come online. The next proposal call—for beam time during the experiment period of December 2011 through May 2012—will close in early September 2011.

Proposals for beam time are reviewed for feasibility, safety, and scientific merit. For more information, see neutrons.ornl.gov/users/proposals.shtml.

Contact: Judy Trimble, trimblejl@ornl.gov

New Scientific Laboratories at SNS

A new complex of laboratories is now open at SNS, providing a flexible, mobile environment where users can work efficiently. The labs, built on the second floor of the SNS Central Laboratory and Office Building, were built with "green" operations in mind, as well as to optimize the available space for researchers' ever-changing scientific needs. With overhead utilities and mobile furniture, the complex's 13 labs allow staff to easily reconfigure the layout of equipment and quickly change an experiment's setup as needed.

"We surveyed more than 900 users on what they needed, and they gave us a wish list," says Chrissi Schnell, scientific laboratory coordinator.

The lab suite provides amenities for testing and includes features such as a cold room, which will be kept at 8°C, outlets and workbenches so that researchers can run equipment for long periods of time, and a furnace closet for solid-state synthesis with a wall with cable management to organize power and gas lines.

The labs also contain standard American Disability Act-compliant fume hoods and safety showers, automatic sliding doors for hands-free access, and a combination of standard and nonstandard power outlets suitable for different instrumentation.

The labs provide a controlled environment for testing new instruments before they go on the beam line. SNS staff have also been working with CNMS to set up a neighboring lab with various x-ray equipment.

Schnell and lab staff will be on hand to provide services to researchers such as chemical management and training. "We are here to meet the needs of the researchers and provide them with excellent customer service," Schnell says.

For more information, see neutrons.ornl.gov/facilities/labs

Contact: Chrissi Schnell, schnellca@ornl.gov

Mike Crawford of DuPont (right), the inaugural user of the new SNS labs, prepares a thin film sample with the assistance of BASIS instrument scientist Souleymane Diallo.

More Precise Data Acquisition Promises More Productive Instrument Time

Event-based data analysis is becoming the standard.

THE SNS PIONEERED THE USE OF EVENT-BASED DATA ACQUISITION, AKA "EVENT DATA," FOR NEUTRON scattering instruments. Event data tracks every neutron that impacts an instrument's detectors and can record the environmental conditions around the sample when the neutron hit.

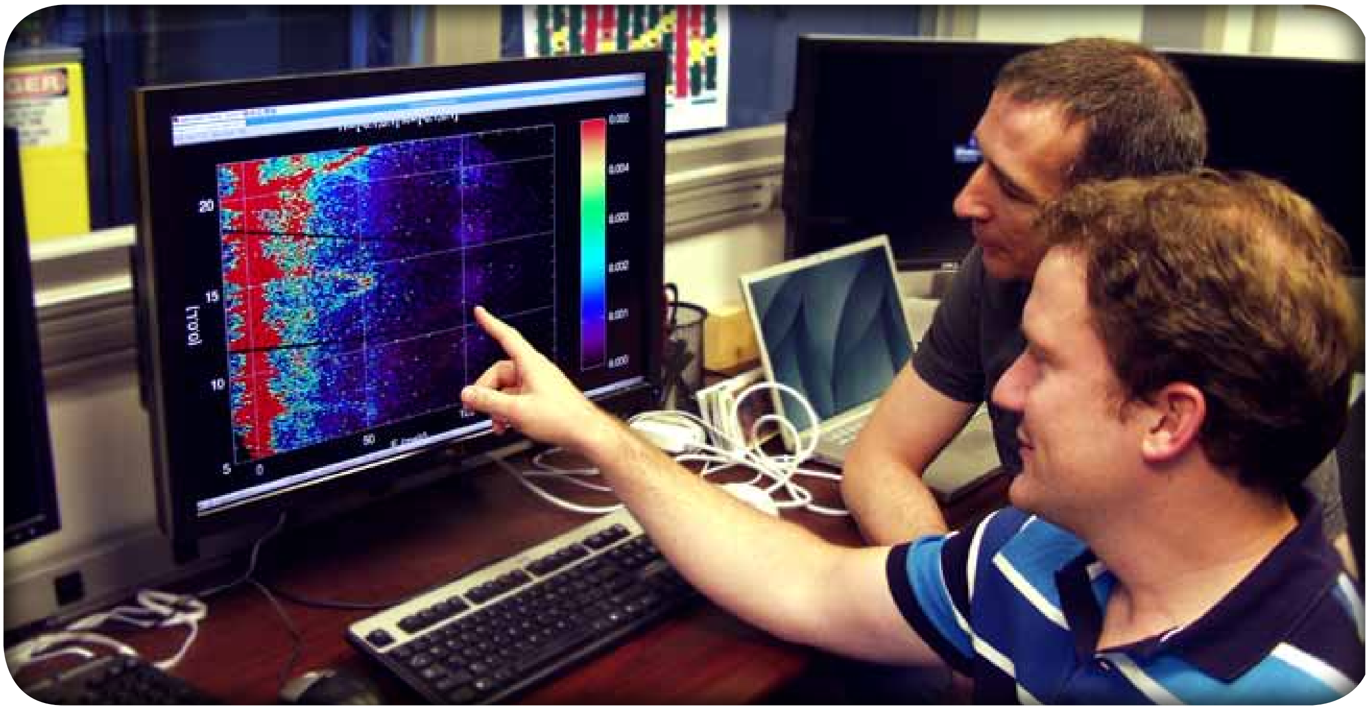
Every SNS instrument has logged neutron impacts using event data mode since SNS came on line. It has taken some time to develop the data analysis tools required to mine and refine the massive event data sets, but users are now beginning to take full advantage of the capabilities the technique presents. The ARCS instrument was an early test-bed for event data analysis (see sidebar), and the techniques are now being used at other instruments, including VULCAN and SEQUOIA.

The traditional method of acquiring scattering data is to sort them into preset "bins" that represent ranges of event position and TOF, explains Steve Miller, leader of the SNS Scientific Data Management group. After an experiment, the data analysis system produces histograms that quantize the data and put them in the closest bin; any resolution information finer than the histogram bin boundaries is lost, Miller says.

Event data mode, however, captures and stores an individual data set for each neutron that strikes the sample—precisely when and where the neutron is detected. This allows the energy, or wavelength, of each detected neutron to be determined from the time-of-flight data. Geometrical information, such as the scattering angle, is ascertained from the three-dimensional arrangement of the detector pixels in the instrument.

"Event data gives researchers the opportunity to process their data at the highest resolution available from the instrument," Miller says. "Better resolution is what it's all about in the world of detecting data.

"We're keeping the maximum amount of information from the experiment at the beginning," explains Doug Abernathy, instrument scientist at ARCS. During analysis, the user can sort the scattering data to pinpoint a particular result and then resort the same data later on to isolate other results. With conventional histogramming, the user must decide before the experiment which subset of data to acquire.



Frank Weber (foreground) and Stephan Rosenkranz of ANL are early adopters of event data analysis at ARCS.

The data acquisition system also can be synchronized with sample environment equipment to collect and store parameters such as temperature, pressure, or magnetic field that are relevant to individual experiments, notes Abernathy.

The SNS design teams considered early on which instruments would benefit from event data mode, Abernathy says. “In the end we decided that all instruments would because it’s almost always an advantage.”

Event data mode is particularly useful for characterizing systems in which structure and/or dynamics (e.g., magnetic order or crystalline structure) are changing rapidly, for example, as a sample is heated or cooled or exposed to electrical or magnetic fields. For example, the technique was valuable in work using a 30-tesla pulsed magnet on SEQUOIA that produced the first-ever neutron scattering results using such a high magnetic field (neutrons.ornl.gov/instruments/SNS/sample/news/PulsedMagnet.shtml).

For event data analysis, instruments must be equipped to write files for every parameter added to an experiment, and users need software that can manipulate all those variables. Event data mode is incorporated into instruments according to the measurement techniques they use. Users of the powder diffractometer POWGEN, for example, won’t care about rotation but might be very interested in magnetic field.

Once the data analysis systems are in full event data mode, as data come in they will flow to analysis tools that will process them and make a plot that updates every second on a screen, Abernathy says. The user will be able to look at the plot and see whether the experiment is going as expected or if something needs to be changed. “If something has gone wrong, you would see it immediately instead of 12 hours later,” he says.

Eventually, SNS staff expect to develop event data analysis tools either in-house or in collaboration with users and make them available to the general user population, Abernathy says.

Contact: Steve Miller, millersd@ornl.gov

Event Data Revolutionizes Measurements of Rotating Crystals

A team consisting of Stephan Rosenkranz, John Paul Castellan, Frank Weber, and Ray Osborn of Argonne National Laboratory (ANL) is among the first to develop the analysis tools to take advantage of event data. With data acquisition and data management staff at SNS, this team pioneered a new technique to efficiently measure broad distributions of inelastic scattering on TOF spectrometers by continuously rotating a crystalline sample during the measurement.

“This particular type of scan is doable only at SNS at this time. In the past, it could not be done because the technology wasn’t there to do and histogram it quickly,” Rosenkranz says.

In conventional data acquisition, recording data at several sample orientations requires something like stop-motion animation: set up the sample at a fixed angle, acquire data for an hour or so, stop, rotate the sample a little bit, and repeat the process for every angle used—a whole series of experiments that can take days, says Rosenkranz. And the researchers wouldn’t know until after the experiment ended whether they had measured the appropriate angles or gotten the data they needed.

The time saved is not the only advantage, and maybe not even the most important. Measuring a limited set of angles risks missing the precise spots where the action is, Rosenkranz explains. Event data mode allows the instrument to sweep across the entire range of possible sample orientations. “Previously, you might measure at the wrong angle—you would measure discrete angles and if you had a very sharp set of excitations, you might miss it. With a sweep, you won’t miss any excitations.”

“With this mode, you can do a quick overview and know what you need to measure, see a picture emerging quickly, and know when you’re measuring what you need to,” he says. “This is a much more efficient way of taking data and getting the most out of your limited beam time.”

In 2014, CORELLI, the Elastic Diffuse Scattering Spectrometer at SNS, will come on line, Rosenkranz notes. It will modulate the neutron beam with a statistical chopper to discriminate among neutrons of different energies. “It will be absolutely crucial for us to have event mode then. CORELLI will have a chopper with many different openings, so the neutrons will have many different flavors. But then you have to know at the end which flavor each neutron has. Event mode data acquisition allows us to do that.”

Users Find Teamwork Instrumental to Success at SNS and HFIR

"If it doesn't agree with the experiment, it's wrong," Richard Feynman, Nobel prize-winning physicist.

IN 2010, NEARLY 800 SCIENTISTS CAME TO SNS AND HFIR TO TEST THEIR RESEARCH THEORIES ON THE FACILITIES' UNIQUE INSTRUMENTS. Each of the 21 available instruments is staffed by a team of instrument scientists and scientific associates, whose work it is to guide users through the experiment that tests their research hypotheses to the successful publication of papers with the relevant data.

Doug Abernathy is the chief instrument scientist for ARCS, which specializes in single-crystal and powder studies in lattice dynamics, magnetic dynamics, and chemical physics.

In 2008, when ARCS was the newest instrument at SNS, an exciting area of research opened up with the discovery of iron-based superconductors. Samples of a new iron arsenide superconductor were brought to ARCS. The measurements taken provided scientists with clear, high-impact data about the phonons and superconductivity in the material. The researchers' paper was published in just three months. "We were partners in figuring out the experiment, running the experiment, and analyzing the data—an example of an extremely tight collaboration," Abernathy recalls.

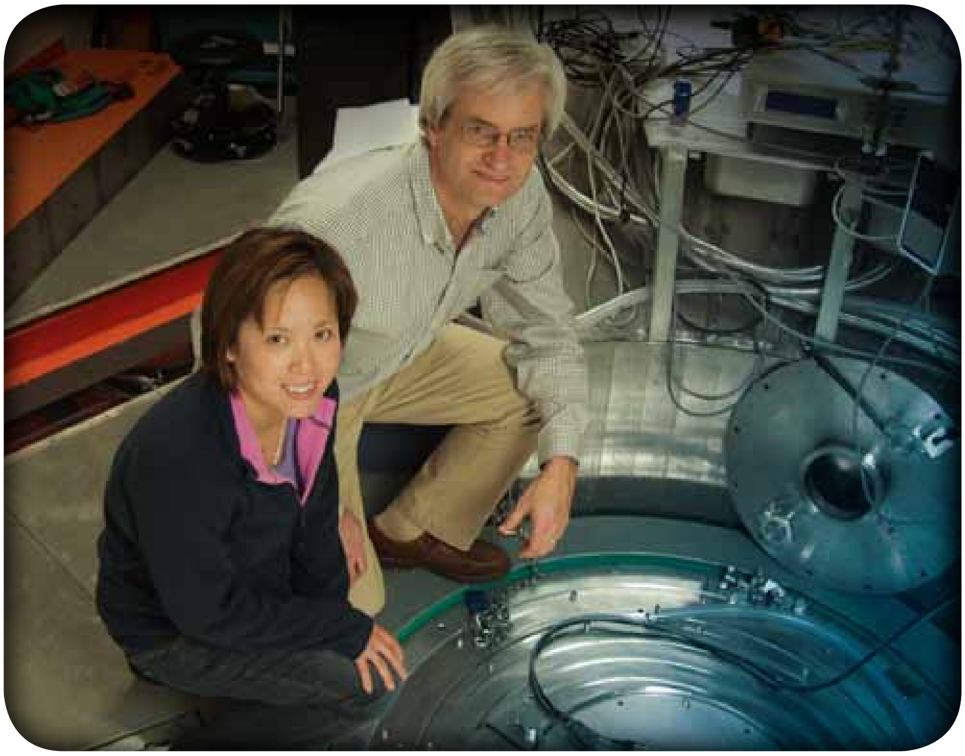
Instrument scientists Abernathy and Matt Stone and scientific associate Mark Loguillo are the go-to ARCS instrument team. When researchers are allocated time on an instrument, one scientist is assigned as the local contact to talk with users about the sample to be studied, its mounting, and any particular safety issues that need to be addressed.

The instrument team deals with a range of competencies. New users need considerable initial guidance and training. Seasoned users need less.

Upon arrival users are shown around the experiment hall and receive radiation protection training and instrument-specific training on things such as logistics and safety.

Before starting an experiment, Abernathy or Stone and the users sit down at the instrument's control computer to discuss how to acquire and reduce data. Users are trained to use the software on the instrument computer to reduce their data so that they can look at it during the experiment and judge how things are going, for example, whether they need to count longer or take more temperature points. "They are then really in control of the experiment and learning new things about the physics in their sample," says Abernathy.

Physicist Ray Osborn and his team at ANL have visited many times. In late 2010, they came to



ORNL Materials Science and Technology researcher Judy Pang and Doug Abernathy, lead instrument scientist for ARCS.

ARCS to do a single-crystal experiment with the superconducting material yttrium nickel boron carbide (YNi_2B_2C). Single crystals are difficult and painstaking to work with, and the time from experiment to published paper is typically 12 months or longer.

"The Osborn group proposed to do a single-crystal experiment with temperatures down to 5 K," Abernathy explains, "a standard piece of sample environment equipment for us." They needed a closed-cycle refrigerator, a type of cooling device. Emails had gone back and forth to ensure that the sample mounting was compatible.

For this experiment the mounting rotated, as the crystal needed a specific orientation relative to the neutron beam. This ensures that when they analyze their data, researchers see the results in a way that they can interpret. The team also wanted to track the rotation angle as the experiment progressed, so they could relate the angle to the data. A lot of interaction was needed to ensure that the right software and hardware were in place.

"We are the tail end of a long process," Abernathy says. "The researchers then take the data and produce their results. We'll see the paper much closer to the end of the process and make some comments about the technical part.

"That is good. It means we are doing our job, supplying the right data."

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The Science at ARCS

ARCS assists research in two broad categories: phonons and magnetism in materials.

Phonons are correlated atomic motions inside a crystal structure. They lead to heat transport and determine sound velocity in a material. They can govern whether crystal structures or some alloy materials are stable. Phonons have certain excitation energies that can be measured using neutron scattering. The applications are particularly relevant for thermoelectric materials, for example, that take heat and convert it to electricity. The behavior of phonons in a thermoelectric material is critical to how effective it is.

Superconductivity has always been the bread and butter of neutron scattering. Researchers study the phonons in a sample to see how they impact its superconductivity. Phonons are integral to other basic questions as well, such as the inter-atomic potential between the atoms in a crystal. The phonon spectrum is a reflection of that potential, of the strength of interactions between the atoms and how it changes at different temperatures in different materials.

ARCS is also ideal for studies in magnetism. Because neutrons have a magnetic moment, they are a good probe of magnetic systems and of the excitations of such systems in materials. With the current SNS power of 1 MW and plans for going higher, smaller samples can be studied in more detail. This is significant as some crystals are difficult to grow and heretofore were not big enough for very small effects to be measured. Such materials can now be revisited and be studied earlier in their development.

ARCS allowed scientists to see the ordered structure of magnetic moments in the new iron arsenide superconductors discovered in 2007 to 2008 and the excitations as the sample evolved through the superconducting transition. It also enabled studies of the effects of chemical doping of certain elements within this superconducting family of materials, which may reveal new information about how magnetism and superconductivity are related.

Experiment Hall Coordinators Are Key to Safe, Smooth Neutron Science

Supporting the user teams and instrument staff in performing wold-class research.

THE HEART OF SNS IS THE EXPERIMENT HALL, AND AT THE HEART OF THIS GIANT CONCRETE AND STEEL bunker of instruments prowled by techies in rumpled t-shirts is the experiment hall coordinator (EHC) team.

There are seven of them—supervisor Terry Collins, Jeff Duff, Dave Dunning, Jack Frye, Kevin Hamby, Tommy Forrester, and Brian Plante—a first-response/safety-first team that, when the neutron scattering instruments are operating and receiving neutrons, work 12-hour shifts around the clock, seven days a week.

“What we do is all about facilitating operations of the neutron scattering instruments and supporting the user teams and instrument staff in performing world-class research,” Collins says.

Experiment Hall Coordinators Kevin Hamby (left) and Jack Frye.

The EHC office overlooks the instrument floor below and allows the EHCs to easily view activity in the hall and the monitors that provide real-time feeds of the status and activity of more than a dozen instruments. EHCs make hourly rounds of the commissioned beam lines to see if there are any issues to be addressed. They ensure safe ambient building temperatures and help coordinate resolution for electrical power outages and other facility utility issues.

The office is also a safety liaison hub between equipment and facility. When a neutron beam interacts with materials in an experiment station, there are potential radiological hazards. Oxygen deficiency hazards are also a factor at some instruments.

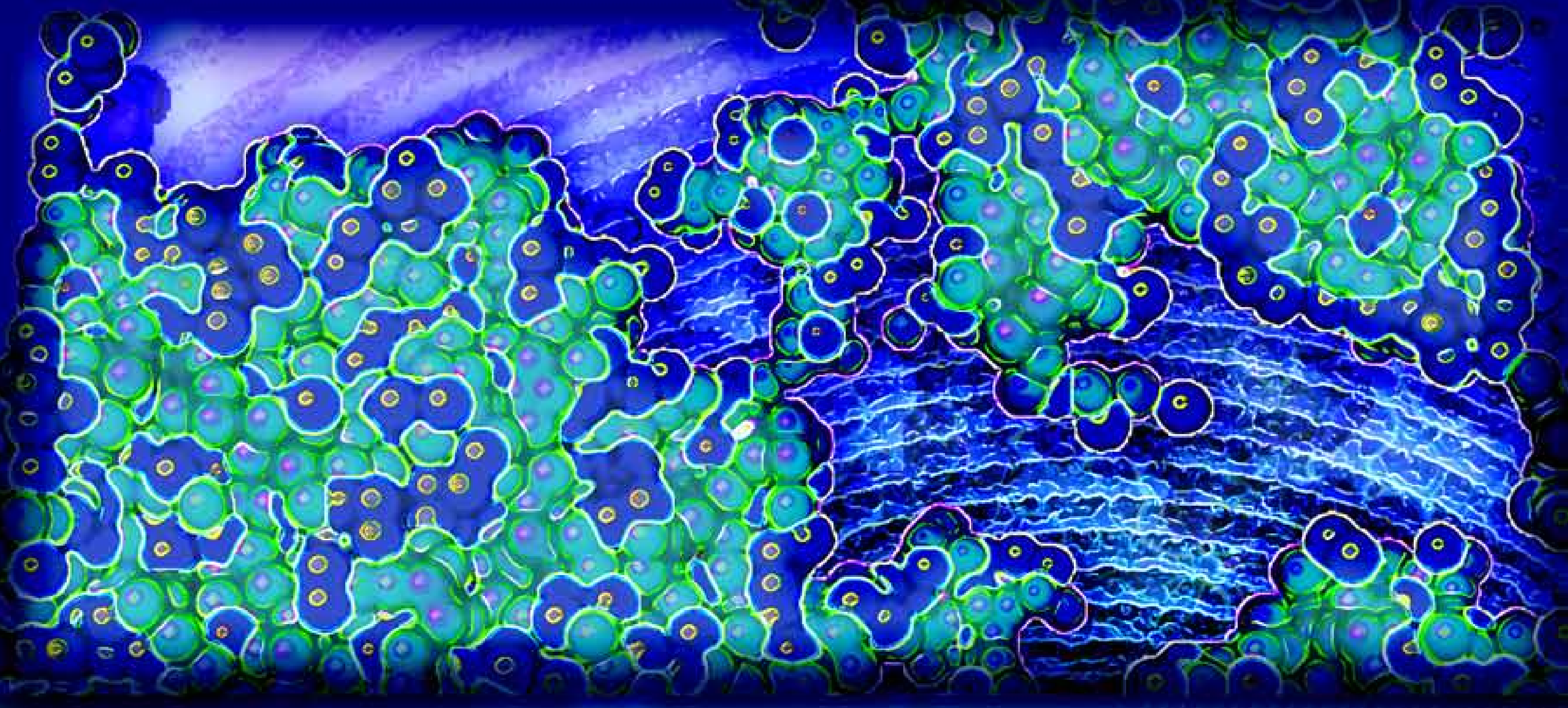
A Personal Protection System is in place to minimize such hazards. Before an instrument can receive neutrons, the team “does a sweep” to account for all staff in the area and completes an extensive checklist of the instrument components to make sure all is clear for the instrument to “take beam.”

“A good analogy would be the checks and signoffs that must be in place before the pilot of a 747 is cleared for takeoff,” says Jack Frye.

During operation, scientists arrive from all over the world. The team gives new users Experiment Hall orientation training, familiarizing them with exits, radiation protection, and numbers to call in case of an emergency.

The EHCs are the main point of contact for all users and staff, and in the deep of night, they’re always there.

Contact: Terry Collins, collinstl@ornl.gov



EDUCATION AND OUTREACH

ONE OF THE TOP PRIORITIES OF THE NEUTRON SCIENCES ORGANIZATION IS EDUCATING SCIENTISTS, students, and the public about scientific and technological advances resulting from neutron research and the possibilities for the future. We hope to motivate members of the science and engineering communities to learn more about the capabilities of neutron scattering in general and the resources available at HFIR and SNS in particular.

Ashfia Huq (front), scientific associate for the SNS Powder Diffractometer, explains neutron diffractometry to teachers participating in the STARs program.

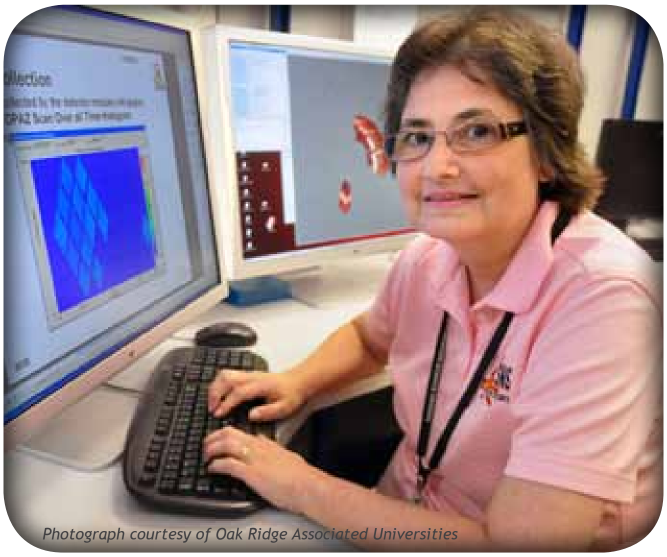
Every year, our staff actively participate in a wide variety of scientific education and outreach activities:

- Hosting or taking part in conference and workshops, including the annual National School on Neutron and X-Ray Scattering
- Presenting educational information at local community events, universities, public schools, and civic meetings
- Training and mentoring postdoctoral fellows, interns, and teachers in the methods and potential of neutron scattering
- Working with the Joint Institute for Neutron Sciences, Oak Ridge Associated Universities, and Oak Ridge Institute for Science and Education
- Developing outreach materials such as publications, displays, multimedia, and the Neutron Sciences Web site
- Providing tours of HFIR and SNS

Development Programs for Teachers

Through ACTS (Academies Creating Teacher-Scientists Professional Development Program), teachers from all over the United States come to ORNL for three consecutive summers to participate in research with leading scientists. The teachers gain valuable knowledge and experience that they can take back to their own schools. The three-year investment gives teachers a sustained opportunity to learn and make a difference at ORNL and with their students back home. In 2010, a physics, math, and computational sciences teacher from Pennsylvania finished her second year working with scientists at the SNS TOPAZ instrument.

Our staff also participated in a new, nationwide program called Siemens Teachers as Researchers (STaRs). This professional development program hosts 20 middle school and high school science and math teachers for two-week research experiences at ORNL. The STaRs program is part of a larger initiative called the Siemens STEM Academy, designed to advance science, technology, engineering, and math (STEM) education in the United States.



Photograph courtesy of Oak Ridge Associated Universities

Elaine Custer, a math and science teacher from Pennsylvania, has worked for the past two summers at the SNS TOPAZ instrument through ACTS.

Shelly Ren (middle), software engineeer for the Scientific Computing Group, with students Brittney Devine (left) and Joaquin Hernandez (right).

Summer intern Mary Beth Parker prepares samples for an experiment at HFIR.

Collaborative Visits and Internships

Throughout 2010, Neutron Sciences hosted 85 students and faculty from all over the United States. Of these, 21 participated in the Collaborative Research Visit Program. Each application for these visits includes a proposed collaborator from ORNL, along with a statement of work outlining the benefit to ORNL. Funds may be provided to foster scientific collaboration with the university scientific community.

Of the students, 67 participated in summer internships, almost double the number for 2009. Prospective interns submit applications for review and are then interviewed. Students selected are assigned to areas suited to their interests and planned career paths, and each student is assigned a mentor responsible for providing learning opportunities and overseeing the student's work.

Visits are arranged through programs such as the

- Oak Ridge Associated Universities Higher Education Research Experiences Program
- DOE National Science Foundation Faculty and Student Teams Program
- ORNL's Nuclear Engineering Science Laboratory Synthesis Program
- DOE-Office of Science undergraduate laboratory internships

Meetings and Workshops

Because not all scientists are familiar with neutron science—specifically neutron scattering science—every year we host or co-sponsor a variety of seminars, meetings, and workshops to educate participants on how neutron scattering can benefit their research. These programs range from workshops focusing on particular neutron scattering techniques to instrument-specific workshops to highlight the capabilities of individual instruments. Last year, we had a very full schedule.

In 2008, ORNL, in collaboration with ANL, began hosting the U.S. National School on Neutron and X-Ray Scattering. During the two-week school, students can perform their own experiments alongside experienced scientists. Students spend one week at Argonne and then travel to ORNL for the second.

Conferences and Workshops Hosted, Organized, or Supported by Neutron Sciences in 2010

Events in Oak Ridge

- Hydrogen and Helium Isotopes in Materials
- IUCr Commission on High Pressure 2010
- National School on Neutron and X-Ray Scattering
- Neutrons for Catalysis
- Neutron Scattering Techniques in Structural Biology
- NOBUGS 2010
- Southeast Regional Collaborative Access Team (SER-CAT) Symposium and Board Meeting
- Summer School in Biophysics at UT/ORNL: Computational and Experimental Challenges
- User Week 2010
- VULCAN (SNS) Instrument Development Team Meeting

Other Co-Sponsored National and International Events

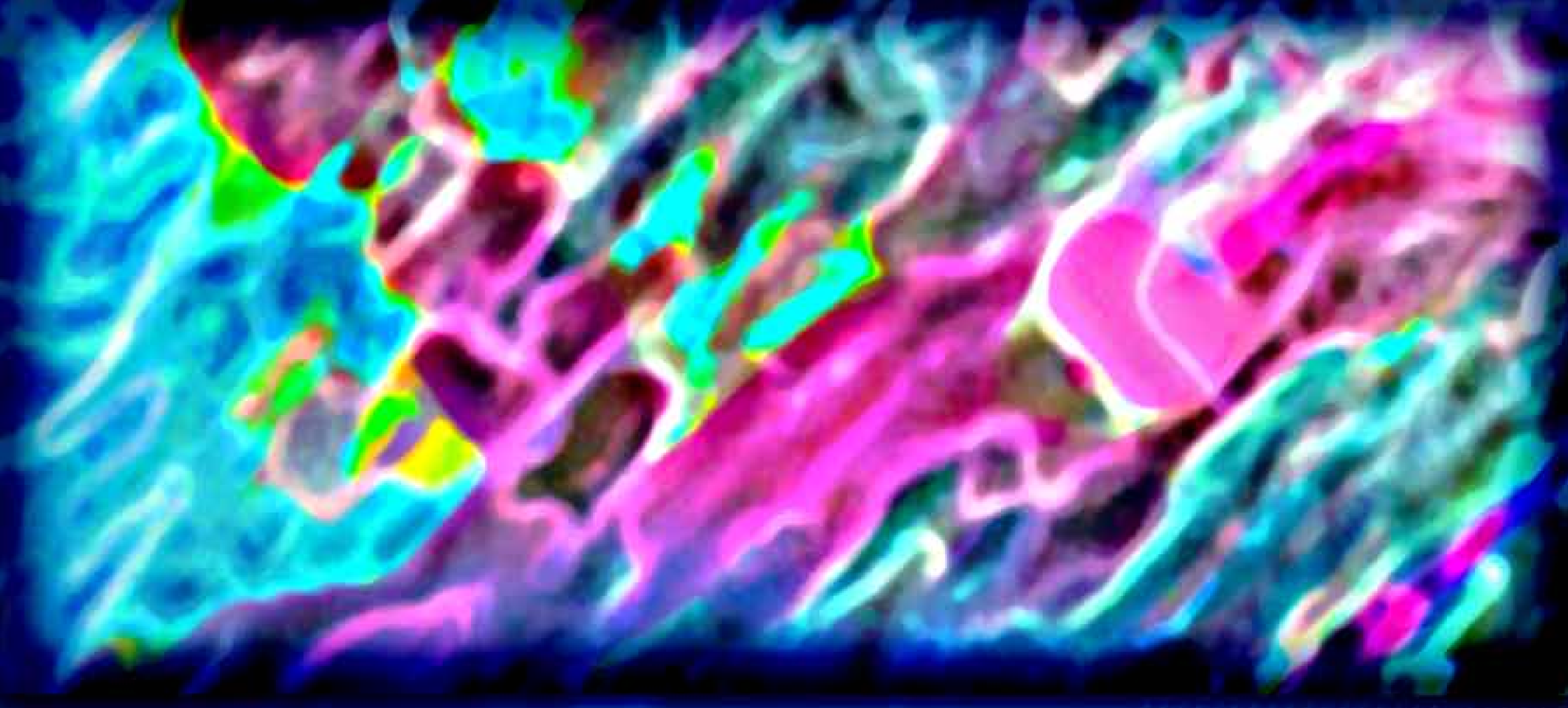
- American Conference on Neutron Scattering 2010, Ottawa, Ontario, Canada
- Highly Frustrated Magnetism 2010, Johns Hopkins University, Baltimore, Maryland, USA
- Neutrons and Food, Sydney, Australia
- Neutrons for Global Energy Solutions, Bonn, Germany

SNS Simulator Exhibit Brings Neutron Science to Kids and Teachers

Perhaps the biggest new educational effort this past year was creation of an "SNS Simulator," a 10 by 30 foot display designed to represent how SNS works. The display is interactive and is targeted at middle school students. It debuted at SNS on National Lab Day and later made appearances at a local career day event for eighth grade students and the inaugural Science and Engineering Festival in Washington, D.C., which hosted an estimated half-a-million visitors. Now requests are pouring in for the simulator to come to other schools.

In the "SNS Simulator," students play the part of an ion beam going through a simulated particle accelerator (left) and then emerge from the exhibit as neutrons, ready to conduct experiments (below). Many adults, notably teachers, also go through the exhibit.

Contact: Al Ekkebus, ekkebusae@ornl.gov



PEOPLE

Neutron Sciences Staff

THE NEUTRON SCIENCES DIRECTORATE IS COMPOSED OF FOUR DIVISIONS, EACH FOCUSED ON A SPEcific mission:

Neutron Facilities Development Division

Neutron Scattering Science Division

Research Accelerator Division (SNS only)

Research Reactors Division (HFIR only)

With a staff of about 640, Neutron Sciences is one of the largest science groups at ORNL. We also participate in a joint faculty appointment system, through which researchers are staff members at both ORNL and partner universities.

HFIR and SNS personnel work with staff from other ORNL research organizations, the Joint Institute for Neutron Sciences, universities, industry, and other research institutes. The goals of these collaborations are to broaden the range and productivity of science programs, promote educational and outreach programs, and ensure the optimum use of ORNL's world-leading neutron facilities.

Community Involvement

Our staff take part in many community outreach activities. During the past year we were involved in ORNL-wide outreach activities such as United Way, Komen Race for the Cure, Buddies Race for the Cure, Juvenile Diabetes Research Foundation walk, Alzheimer's Association Memory Walk, Tour de Cure for the American Diabetes Association, Coats for the Cold, Christmas Collection for the Needy Elderly, and the Angel Tree program.


Allison Orcutt, Katie Smith, and Megan Scott at the Komen Race for the Cure.


Tenth annual Collection for the Needy Elderly.

In addition to ORNL-sponsored events, various groups participated in the National Gaucher Foundation Walk and Car Show; Knox Area Rescue Ministries; Ecumenical Storehouse ministry; Friends of Literacy; American Youth Soccer Organization; Willow Brook Baptist Church "Thanksgiving Away" benefit; Mission of Hope, which delivers backpacks and Christmas toys to Appalachian schools; and various programs to help the homeless, scouting programs, and sports leagues for special-needs children. HFIR staff also served on a flood relief team in Nashville, Tennessee.

Honors and Awards

Xun-Li Wang was elected fellow of the American Physical Society for "sustained contribution in neutron diffraction studies of structure, phase transformations, and mechanical behavior in materials and engineering systems and leadership in the design and construction of a versatile engineering diffractometer at SNS."

Herbert Mook was awarded the 2010 Clifford G. Shull Prize from the Neutron Scattering Society of America. Mook was cited for "outstanding contributions to the study of magnetism, superconductivity, and quantum phenomena in matter with neutrons."

HFIR employees brought their families to tour the complex during HFIR Family Day in September.

Steve Nagler was elected fellow by both the American Association for the Advancement of Science and the Neutron Scattering Society of America.

Yang Zhang was named the 2010 Shull Fellow. He is investigating the physics of fluids, glasses, and soft materials using neutron scattering and high-performance computing simulation at ORNL.

Richard Riedel, Ronald Cooper, and Lloyd Clonts received an Excellence in Technology Transfer Award for development of a Position-Sensitive Detector Electronics System and Neutron Detector Assembly. The award was given by the Federal Laboratory Consortium, Southeast Region.

Sam McKenzie (right) receives the Director's Award for Community Service at the annual ORNL Awards Night. On the left is ORNL Director Thom Mason.

Powder Diffraction Group leader Xun-Li Wang shows his daughter around HFIR.

Mike Simonson and John Katsaras were named senior scientists in the Neutron Scattering Science Division.

Fabio Casagrande was elected to the Cryogenics Society Board.

In recognition of excellence in science communications, Deborah Counce, Charlie Horak, Reneé Manning, and Genevieve Martin received a silver award in the Magnum Opus Custom Media competition and three awards from the Society for Technical Communication.

Sam McKenzie received the ORNL Director's Award for Community Service. McKenzie was cited for "excellence in community leadership throughout East Tennessee."

Contact: Al Ekkebus, ekkebusae@ornl.gov

Advisory Committees

Neutron Sciences Advisory Board

Chair, Meigan Aronson, Brookhaven National Laboratory

The Advisory Board reports to the ORNL director and advises the associate laboratory director for Neutron Sciences on all aspects of ORNL's neutron facilities. The goal of the committee is to maximize the scientific impact and benefit of these facilities to ORNL, DOE, and the national and international scientific communities. The committee identifies, and brings to attention of laboratory management, issues critical to the technical and scientific success of ORNL neutron facilities, including meeting performance, cost, and schedule goals. The committee is made up of members of the scientific communities that are fundamentally involved with HFIR and SNS, as well as individuals with experience managing major science facilities, particularly materials research facilities.

Neutron Scattering Science Advisory Committee

Chair, Susan Krueger, National Institute of Standards and Technology

This committee reports to the associate laboratory director for Neutron Sciences and advises NSSD and Neutron Facilities Development Division (NFDD) directors on the directorate's science programs and instrument development. Primarily, the committee provides advice on the types of instruments required to effectively meet the requirements of a multidisciplinary scientific community. The committee also counsels the NSSD director on outreach programs and interaction with the neutron user community. Committee members consist mainly of members from the scientific community who are experts in the instrumentation at HFIR and SNS, potential users, and managers with experience in the effective operation of user programs.

SNS Accelerator Advisory Committee

Chair, Gerry Dugan, Cornell University

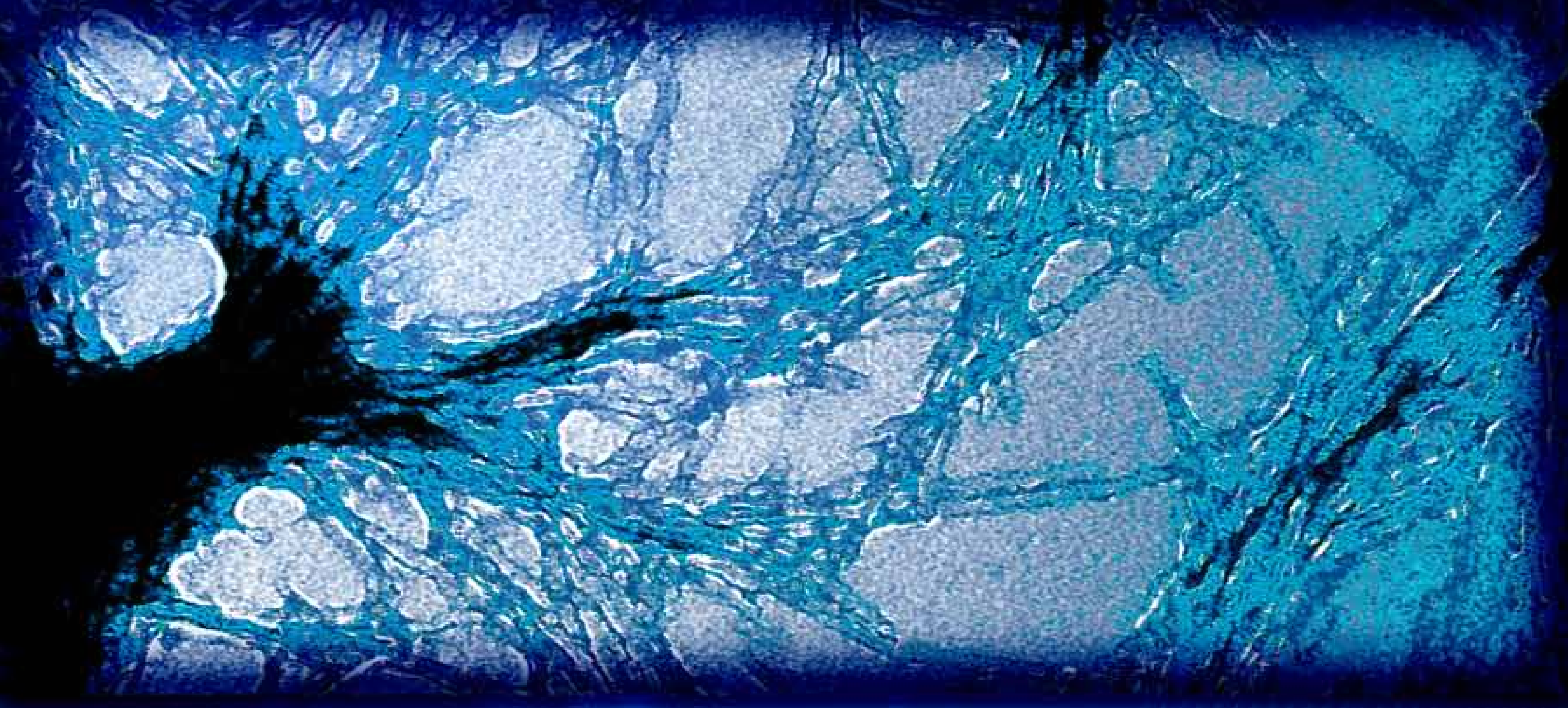
This committee reports to the associate laboratory director for Neutron Sciences and advises the Research Accelerator Division (RAD) and NFDD directors on the operations and performance of the SNS accelerator complex. Committee members are appointed by the Neutron Sciences associate laboratory director in consultation with the RAD and NFDD directors.

Instrument Advisory and Development Teams

Instrument advisory teams work with the ORNL staff to design and construct instruments funded by ORNL Neutron Sciences. These instruments are made available to the user community through a peer-reviewed proposal system. Instrument development teams (IDTs) build, and sometimes operate, instruments funded from other sources. A portion of beam time on these instruments is allotted for the scientific program of the IDT, with the balance available for general users. At least 75% of the beam time for these instruments is devoted to the general user program. Policies and guidelines regarding instrument development and use are available at neutrons.ornl.gov/users/policies.shtml.

SNS-HFIR User Group Executive Committee

SHUG was formed to provide a link between the neutron scattering community at ORNL and the management of SNS, HFIR, and JINS. SHUG also serves as an advocacy group for SNS and HFIR. The Executive Committee is composed of a rolling membership of 12 distinguished individuals from the neutron science community. Cora Lind, University of Toledo, is serving as the current chair. For more about the user program, see p. 54.



ACRONYMS AND ABBREVIATIONS

Acronyms and Abbreviations

Å	angstrom
ARCS	Wide Angular-Range Chopper Spectrometer
ACTS	Academies Creating Teacher-Scientists Professional Development Program
ANL	Argonne National Laboratory
BASIS	Backscattering Spectrometer
Bio-SANS	Biological Small-Angle Neutron Scattering (instrument)
C	Celsius
CNCS	Cold Neutron Chopper Spectrometer
CNMS	Center for Nanophase Materials Sciences
CO_2	carbon dioxide
CORELLI	Elastic Diffuse Scattering Spectrometer
CSM	central solenoid magnet
CSMB	Center for Structural Molecular Biology
CTAX	Cold Triple-Axis Spectrometer
CVI	chemically vapor infiltrated
DOE	U.S. Department of Energy
dpa	displacements per atom
DPF	diesel particulate filters
EC	executive committee (SHUG)
ECBM	enhanced coal bed methane
EFRC	Energy Frontier Research Center
EGR	exhaust gas recirculation
EHC	Experiment Hall coordinator
EPRI	Electrical Power Research Institute
EQ-SANS	Extended Q-Range Small-Angle Neutron Scattering Diffractometer
FEERC	Fuels, Engines, and Emissions Research Center
Fe SC	iron-based superconductor
FeSi	iron silicide
FNPB	Fundamental Neutron Physics Beam Line
GB	gigabyte
GeV	gigaelectronvolt
^{3}He	helium-3
HFIR	High Flux Isotope Reactor
HNLS	Hi-Nicalon™ Type-S
HPSS	High-Performance Storage System
HTML	High Temperature Materials Laboratory
HTS	high-temperature superconductors
HYSPEC	Hybrid Spectrometer
Hz	hertz
IDT	instrument development team
IMAGINE	Image-Plate, Single-Crystal Diffractometer
INS	inelastic neutron scattering
ITER	International Thermonuclear Experimental Reactor
JINS	Joint Institute for Neutron Sciences
K	kelvin
kg	kilogram
km	kilometer
kW	kilowatt
La_3Te_4	lanthanum telluride
lb	pound
^{6}Li	lithium-6
MaNDi	Macromolecular Diffractometer
m	meter
MeV	megaelectronvolt
mg	milligram
μm	micrometer
MIT	Massachusetts Institute of Technology
MTSU	Middle Tennessee State University
MW	megawatt
NASA	National Aeronautics and Space Administration
NCCS	National Center for Computational Sciences
NCSU	North Carolina State University

NFDD	Neutron Facilities Development Division
NIST	National Institute of Standards and Technology
nm	nanometer
NMR	nuclear magnetic resonance
NRC	1. Nuclear Regulatory Commission 2. National Research Council of Canada
NO_x	nitrogen oxide
NOMAD	Nanoscale-Ordered Materials Diffractometer
NSE	Neutron Spin Echo Spectrometer
NRSF-2	Neutron Residual Stress Facility
NSSD	Neutron Scattering Science Division
ORISE	Oak Ridge Institute for Science and Education
ORNL	Oak Ridge National Laboratory
PAMAM	polyamidoamine dendrimers
PbTe	lead telluride
PFS	porous fractal silica
POWGEN	Powder Diffractometer
PWR	pressurized water reactor
QENS	quasielastic neutron scattering
RAD	Research Accelerator Division
RRD	Research Reactors Division
s	second
SANS	small-angle neutron scattering
SEQUOIA	Fine-Resolution Fermi Chopper Spectrometer
SHaRE	Shared Research Equipment User Facility
SHE	superheavy element
SiC	silicon carbide
SHUG	SNS-HFIR User Group
SNAP	Spallation Neutrons and Pressure Diffractometer
SNS	Spallation Neutron Source
StaRs	Siemens Teachers as Researchers
STEM	science, technology, engineering, and math
T	tesla
TB	terabyte
TOF	time of flight
TOPAZ	Single-Crystal Diffractometer
USANS	Ultrasmall-Angle Neutron Scattering
VISION	Chemical Spectrometer
VULCAN	Engineering Materials Diffractometer
YNi_2B_2C	yttrium nickel boron carbide

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