

Oak Ridge National Laboratory Neutron Sciences Progress Report December 2010

Neutron Highlights

The deadline for the next [call for HFIR and SNS proposals](#) is **February 23, 2011**, for the June–November 2011 period.

Applications for the 2011 **National School on Neutron and X-ray Scattering** are being accepted. The NXS School will be held June 12–25, 2011 at Argonne and Oak Ridge. Applications are due February 28, 2011. [Details](#)

At HFIR, Cycle 432 ended December 17, 2010, and Cycle 433 began January 10, 2011. The HFIR long-term schedule is [available](#).

At SNS, the current cycle of neutron production ended December 20, 2010, and will resume February 14, 2011. The detailed SNS schedule is [available](#). Recent availability is approaching 95%.

Science Highlights

SANS maps protein distribution in silica matrix for novel biotech applications. Researchers at ORNL, in collaboration with the Air Force Research Laboratory, have investigated the properties of a novel composite material with antimicrobial properties that is formed by lysozyme-templated precipitation of silica synthesized by sol-gel chemistry. Biomineralization reactions, common in nature, have become a versatile tool for nanobiotechnology. Understanding how proteins interact with the silica matrix is key to optimizing this process for practical applications. Small-angle neutron scattering (SANS) experiments, carried out at ORNL's High Flux Isotope Reactor, were combined with electron microscopy analysis to clarify the assembly and organization of the lysozyme–silica composite material 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. It was determined that the lysozyme molecules are spatially correlated in the material and form clusters with colloidal silica particles. The size of the clusters determined by SANS agrees well with the structural architecture observed by transmission electron microscopy. “Protein localization in silica nanospheres derived via biomimetic mineralization,” M. B. Cardoso, H. R. Luckarift, V. S. Urban, H. O’Neill, G. R. Johnson, *Advanced Functional Materials* **18**(20), 3031–3038, September 23, 2010.

Neutron scattering reveals Einstein modes in the thermoelectric material $\text{Yb}_{0.2}\text{Co}_4\text{Sb}_{12}$. Researchers at ORNL's Spallation Neutron Source (SNS) and Brookhaven National Laboratory have investigated the properties of the thermoelectric material $\text{Yb}_{0.2}\text{Co}_4\text{Sb}_{12}$ and found evidence of Einstein oscillator modes at low and intermediate phonon energies. Thermoelectric materials develop an electric potential in response to a temperature difference across their surfaces and are highly sought after for possible industrial use. Inelastic neutron scattering experiments carried out on the Cold Neutron Chopper Spectrometer at the SNS, combined with specific-heat measurements, provide compelling evidence for the existence of an Einstein oscillator (rattler) mode at $\omega_{E1} \sim 5.0$ meV in the filled skutterudite $\text{Yb}_{0.2}\text{Co}_4\text{Sb}_{12}$. Multiple dispersionless modes in the measured density of states of $\text{Yb}_{0.2}\text{Co}_4\text{Sb}_{12}$ at intermediate energy transfers ($14 < \omega < 20$ meV) are exhibited in both the experimental and theoretical density of states of the Yb-filled specimen. A peak at 12.4 meV is shown to coincide with a second Einstein mode at $\omega_{E2} \sim 12.8$ meV obtained from heat-capacity data. Increasing the understanding of these intermediate energy modes is likely to demonstrate the importance of filler atoms in filled skutterudite thermoelectric materials and allow the development of more efficient thermoelectric materials. “Einstein modes in the phonon density of states of the single-filled skutterudite $\text{Yb}_{0.2}\text{Co}_4\text{Sb}_{12}$ ” I. K. Dimitrov, M. E. Manley, S. M. Shapiro, J. Yang, W. Zhang, L. D. Chen, Q. Jie, G. Ehlers, A. Podlesnyak, J. Camacho, and Qiang Li, *Physical Review B* **82**, 174301, November 2010.

SANS team finds structural differences in virus particles from different host species. A research team using small-angle neutron scattering (SANS) at DOE's High Flux Isotope Reactor at ORNL has demonstrated for the first time that particles of the *Sindbis* virus from insect and mammalian hosts exhibit subtle structural differences. The *Sindbis* virus (discovered in 1952 in Cairo, Egypt) is transmitted from birds (vertebrate hosts) by mosquitoes (invertebrate vectors) to humans (vertebrate mammalian hosts), causing Sindbis fever, which is accompanied by joint pain, rash, and malaise. The scattering data and modeling 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 demonstrated 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. The complex natural cycle of vectored viruses that transition between host species, such as insects and mammals, makes understanding the full life cycle of the virus a difficult challenge. This is the first study in which the structural differences between particles of *Sindbis* viruses grown in mammalian and insect cells were determined by SANS, a nondestructive technique that did not decrease the infectivity of the probed *Sindbis* virus particles. The study received the 2010 Best LDRD Project Award at ORNL. "The structure of *Sindbis* virus produced from vertebrate and invertebrate hosts determined by small-angle neutron scattering," L. L. He, A. Piper, F. Meilleur, D. A. A. Myles, R. Hernandez, D. T. Brown, and W. T. Heller, *J. Virol.* **84**: 5270–5276 (2010).

New or Expanded Capabilities



The Vibrational Spectrometer (VISION) is under construction at SNS BL-16B and commissioning is to begin in 2012. The upper floor (see image at left) is where the sample environment will be loaded into the spectrometer and samples will be changed. Users will work on the upper floor with equipment needed to monitor, control, or manipulate their samples. The second floor will not be accessible when beam is on the sample. VISION can be thought of as the neutron analogue of an infrared-Raman spectrometer. It is optimized to characterize molecular vibrations in a wide range of crystalline and disordered materials over a broad energy range (<5 to >500 meV) while simultaneously recording structural changes using diffraction detectors in the backscattering position and at 90° . This inverted-geometry instrument offers enhanced performance by coupling a white beam of incident neutrons with two banks of 7 analyzer modules, equipped with time and spatially focused crystal arrays that select and concentrate the desired neutrons on a small detector. This arrangement leads to improved signal to noise ratio and a high overall count rate in the inelastic signal compared with currently available similar spectrometers. Christoph (Uli) Wildgruber, wildgruber@ornl.gov, is the VISION instrument scientist.

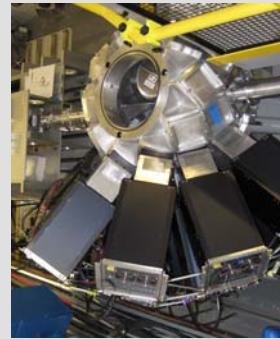


Construction has begun on CORELLI, an elastic diffuse scattering spectrometer on SNS BL-9; commissioning is scheduled for 2014. CORELLI is a statistical chopper spectrometer with energy discrimination. The momentum transfer ranges from 0.5 to 12 \AA^{-1} , and the energy of incident neutrons ranges from 10 to 200 meV. This instrument combines the high efficiency of white-beam Laue diffraction with energy discrimination by modulating the beam with a statistical chopper. A cross-correlation method is used to reconstruct the elastic signal from the modulated data. Accurate modeling of the short-range order associated with the diffuse scattering requires measurements over large volumes of three-dimensional reciprocal space, with sufficient momentum resolution to distinguish the diffuse signal from the strong Bragg peaks. CORELLI is designed and optimized to probe complex disorder in crystalline materials through diffuse scattering of single-crystal samples. Studies at this instrument encompass a wide range of novel materials: colossal magnetoresistance materials, ferroelectric relaxors, fast ion conductors, high-temperature superconductors, geometrically frustrated systems, quantum critical phenomena, and molecular solids and microporous framework systems. Feng Ye, yef1@ornl.gov, is the CORELLI instrument scientist.

First user of SNS labs. Mike Crawford, a chemist at DuPont who's a regular at SNS and HFIR, was the first outside user to take advantage of the new SNS second-floor laboratory suite. [See the highlight.](#)

Research in quantum fluids and solids at SNS. Sample environment capabilities for low-temperature research at the SNS are expanding through a combination of off-the-shelf equipment purchases and development of new devices and techniques. These added capabilities are attracting and enabling a number of research projects in the field of quantum liquids and solids at the facility. Of particular importance is the recently commissioned cryogen-free dilution refrigerator (with $300 \mu\text{W}$ cooling power at low temperatures) that is now available for the users program. The cryostat has already been used reliably at ARCS and CNCS to investigate the dynamics in liquid and solid ^4He at low temperatures, reaching a base temperature of 38.5 mK.

The TOPAZ time-resolved Laue single crystal diffractometer (SNS BL-12) has successfully measured the first user samples during its commissioning phase and is entering the user program in spring 2011. The diffractometer is equipped with 14 neutron area detectors, which make it possible to collect a hemisphere of data in one to two days. The instrument accommodates interchangeably a nitrogen cold-flow for cooling a sample to 100 K, and a helium closed-cycle refrigerator capable of cooling to 5 K. TOPAZ has already shown great versatility for user experiments in structural studies of a vitamin B12 derivative, Li-ion battery materials, shape memory intermetallics, magnetic phase transition in a multiferroic single crystal, and functional thin films. Instrument improvement continues in the upcoming neutron beam cycle, along with installation of a sample cell for gas adsorption and separation in metallic organic framework materials and testing of a ^3He incident beam polarizer for a magnetic structure determination. A "fitting test" of the polarizer at the TOPAZ beam line was conducted successfully. Christina Hoffmann, hoffmanncm@ornl.gov, and Xiaoping Wang, wangx@ornl.gov, are the TOPAZ instrument scientists.



View of the TOPAZ detector array with detectors attached at the end of the incident beam path.

Brief Items about Instruments, People, and Users

Three ORNL neutron scattering users were recently named **Fellows** of the **American Physical Society**: Robert McQueeney, Iowa State University (development and use of neutron scattering techniques to advance the understanding of strongly correlated electron systems), Dave Christen, ORNL (sustained discovery and leadership in understanding of superconductive materials, especially their current conduction and vortex state properties), and Xun-Li Wang, ORNL (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 the Spallation Neutron Source).

Among the five people selected by **The Minerals, Metals & Materials Society** (TMS) for the 2011 **Class of Fellows** is ORNL's Steven Zinkle, who uses HFIR to study radiation effects on materials.

University of Tennessee and ORNL scientists have moved into the **Joint Institute for Neutron Sciences**. A formal ribbon cutting was held December 3, 2010.

Mike Simonson and John Katsaras have been named **senior scientists** in the Neutron Scattering Science Division.

Publication citations are needed for reports to our sponsor and for selection of annual report highlights. [Send](#) us the citation if your publication is not included on our [lists](#). There is a standard [acknowledgment](#) for HFIR or SNS experiments. Let us know if research here contributed to your thesis.

The **2011 U.S. National School on Neutron and X-ray Scattering** is scheduled for June 12–18, 2011, at Oak Ridge and June 18–25, 2011, at Argonne, Illinois. Details are available at the School's [Web site](#). It is funded by the U.S. Department of Energy's Office of Basic Energy Science. Pdfs of notes (all) and videos (neutron portion only) of the lectures are [available](#).

There are [collaborative research opportunities available](#) at HFIR and SNS, including short- and long-term research placements for university-based postdoctoral fellows and graduate students to pursue research using neutron scattering at ORNL. These include visiting student thesis, postdoctoral research, and faculty sabbatical programs.

New "End of Experiment" report requirement. The neutron scattering science program at ORNL is initiating an End of Experiment (EoE) report requirement. For completed experiments, the principal investigator will receive an EoE notification e-mail with details for submitting the report directly via the proposal system (using the pen and pad icon on the dashboard). Contact the User Office at neutronusers@ornl.gov or 865-574-4600 for questions or additional information.

[Travel grants](#) are available through The University of Tennessee for faculty and students from institutions in [EPSCoR states](#) to carry out approved experiments at HFIR or SNS and for travel to discuss experiments before and after the measurements. Contact [Hope Moore-Webb](#) for details.

The [National User Facility Organization](#) reports that participants at U.S. national user facilities—such as synchrotron and neutron, nanoscience, high-energy and nuclear physics, microscopy, and astronomy facilities—now total more than 25,000.

Employment Opportunities

Positions in the Neutron Sciences Directorate or related to neutron scattering. Click on “View Open Positions” at <http://jobs.ornl.gov/> and view Position Category noted as “Science—Neutron Science.”

- Clifford G. Shull Fellowship Program (NC50243236)
- Detector Scientist (NC50256548)
- Extended Q-Range Small-Angle Neutron Scattering (EQ-SANS) Instrument Scientist (NC50252351)
- Neutron Sciences Industrial Liaison (NC50235889)

Collaborative Research Visits Program, including Visiting Student Thesis Research, Visiting Postdoctoral Research, and Faculty Research Sabbaticals; see <http://neutrons.ornl.gov/crv/>.

Fellowship positions with ORNL through Oak Ridge Associated Universities. Descriptions are available at <http://www.ornl.gov/orise/edu/ornl/postneeds.htm>. Recently announced open positions are

- [Post-Masters Associate for the Bio-SANS Instrument](#) (ORNL11-28-NSSD)
- [Magnetism Reflectometer Research Scientist—Career Development Program](#) (ORNL11-27-NSSD)
- [Postdoctoral Research Associate in Neutron Imaging Research—Career Development Program](#) (ORNL11-19-NSSD)
- [Postdoctoral Research Associate—Instrument Development Group](#) (ORNL11-18-NFDD)
- [Postdoctoral Research Associate for In-situ Neutron Scattering Studies of Fuel Cell Materials](#) (ORNL11-16-NSSD)
- [Postgraduate Research Associate in Optical Engineering](#) (ORNL11-10-RAD)
- [Postdoctoral Research Associate in Neutron Spin Filters](#) (ORNL11-06-NFDD)
- [Postdoctoral Research Associate in Neutron Diffraction and Small Angle Scattering Studies](#) (ORNL10-152-CSD)
- [Postgraduate Instrument Associate in the ToF Inelastic Group](#) (ORNL10-141-NSSD)
- [Neutron Scattering Instrument Scientist](#) (multiple positions) (ORNL10-139-NSSD)
- [Postdoctoral Research Associate in Neutron Scattering](#) (ORNL10-137-NSSD)
- [Postdoctoral Research Associate in Computational Nuclear Engineering and Materials Irradiation](#) (ORNL10-136-RRD)

Educational and Research Experiences

ORNL has educational programs covering many scientific disciplines with an education continuum from pre-college through postgraduate, including teachers and faculty. The main link to all of these programs is <http://www.ornl.gov/orise/edu/ornl/>.

Applications are open now for summer 2011 programs.

Meetings and Other Events of Interest to SNS and HFIR Users

February 17–21, 2011. [2011 American Association for the Advancement of Science Annual Meeting](#), Washington, D.C. ORNL is participating in booth 420 and is sponsoring an exhibitor’s forum with Argonne National Laboratory on [“Integrated resources: a competitive advantage of DOE national laboratories.”](#) 3:30–4:30 pm on Friday, February 18, in room 158AB, Washington Convention Center. Abstract: User facilities at U.S. Department of Energy (DOE) national laboratories offer tremendous capabilities for multidisciplinary scientific research using x-ray, neutron, microscopy, and nanoscale techniques. The specialized instrumentation and expertise available at these facilities enable scientists from academia, industry, and other organizations to conduct experiments with resources typically not available at their home institutions. Additionally, the co-location of many of these facilities offers opportunities for the use of multiple techniques or probes on a single sample or group of samples. The goal of this workshop is to describe and promote the competitive advantages of conducting scientific research at these DOE user facilities. Workshop presenters: Brian Toby, Argonne National Laboratory; Malcolm Guthrie, Carnegie Institution of Washington; and Joseph Ng, University of Alabama–Huntsville.

February 23–25, 2011, [Neutron Applications on Strongly Correlated Electron System 2011 \(NASCES11\)](#), Tokai, Japan

March 10-11, 2011. [WKU Nondestructive Analysis \(NOVA\) Center](#), Western Kentucky University, Bowling Green, KY

April 16–18, 2011, **SANS data reduction and analysis workshop**, Oak Ridge, Tennessee

The goal is to assist past users in reducing and mostly analyzing data collected at Bio-SANS and GP-SANS since 2007. Attendance is limited at this workshop; participation is directed to past users who have data that have not been reduced, analyzed, or published. Contact Lisa Debeer-Schmitt, debeerschmlm@ornl.gov, for more information.

May 23–27, 2011, [2nd course on Neutron Scattering Applications in Structural Biology](#), Oak Ridge, Tennessee
The course will include a symposium, lectures and tutorials, and tours of the High Flux Isotope Reactor and Spallation Neutron Source, the world's leading neutron research facilities. The course is designed for graduate students with knowledge of protein function and structure but limited or no experience in the neutron sciences. Application deadline is March 31, 2011.

May 28–June 2, 2011, [American Crystallographic Association](#), New Orleans, Louisiana
There are many sessions related to use of neutron scattering across the broad crystallographic sciences.

June 11–25, 2011, [Thirteenth National School on Neutron and X-ray Scattering](#), Oak Ridge, Tennessee, and Argonne, Illinois
The main purpose of the National School on Neutron and X-ray Scattering is to educate graduate students on the use of major neutron and x-ray facilities. Lectures—presented by researchers from academia, industry, and national laboratories—will include basic tutorials on the principles of scattering theory and the characteristics of the sources, as well as seminars on the application of scattering methods to a variety of scientific subjects. Students will conduct short experiments at Argonne's Advanced Photon Source and Oak Ridge's SNS and HFIR to gain hands-on experience in using neutron and synchrotron sources. Applications are due February 28, 2011. Details are available at <http://www.dep.anl.gov/nx/>.

June 21–23, 2011, Workshop on the TOPAZ Single Crystal Diffractometer, Oak Ridge, Tennessee
Contact Christina Hoffmann, hoffmanncm@ornl.gov, for more information.

October 30–November 4, 2011, [AVS 58th Annual International Symposium and Exhibition](#), Nashville, Tennessee

Future proposal call dates for HFIR and SNS:

February 23, 2011, midnight, Wednesday: proposals for the period June–November 2011

September 14, 2011, midnight, Wednesday: proposals for the period December 2011–May 2012

February 29, 2012, midnight, Wednesday: proposals for the period June–November 2012

Neutron Science in the News

Modern Marvels Secret Undergrounds

The episode on the History Channel includes SNS.

Dr. Know (WBIR, 1/10/2011)

The segment featured Chris Stanley and research at Bio-SANS that is providing insight into the mechanisms of Huntington's disease.

4 ORNL scientists named American Physical Society Fellows (Eurekalert, 12/17).

OAK RIDGE, Tennessee, December 17, 2010—Four researchers from the Department of Energy's Oak Ridge National Laboratory have been elected to fellowship in the American Physical Society. David Christen, David Geohegan, Xun-Li Wang, and William Weber were named APS fellows in recognition of their outstanding contributions to physics.

leading science labs collaborate on open source software (Benzinga, 12/10).

Oak Ridge National Laboratory and Rutherford Appleton Laboratory neutron source scientists team up with Tessella to deploy open source software solution for international data reduction and analysis project

Frank Munger: UT ORNL commitment survived tough economy (Knoxville News Sentinel, 12/8).

More than a decade ago, the state made a commitment to spend \$18 million to build three institutes at [Oak Ridge National Laboratory](#). That commitment was contingent on the University of Tennessee's winning the contract—along with Battelle Memorial Institute—to manage the federal research lab.

Dr. Know (WBIR, 12/8/2010).

Dr Know of ORNL describes researching how to make switchgrass into an economical fuel for your car.

State's tab for joint institutes at ORNL: \$32.1M (Knoxville News Sentinel, 12/6).

As part of a commitment made a decade ago to help the University of Tennessee land its new role in managing ORNL, the state funded construction of three joint institutes—the final one of which (the Joint Institute for Neutron Sciences) was dedicated .

[Another record at Spallation Neutron Source \(Knoxville News Sentinel, 12/3\)](#). Ian Anderson, associate lab director at Oak Ridge National Laboratory and director of the Spallation Neutron Source, said the SNS set a new milestone on Thursday. "We ran the spallation source at 100 percent reliability at a megawatt," Anderson said today following a dedication ceremony at the Joint Institute for Neutron Sciences (just down the hill from the SNS).

[Bredesen dedicates joint research facility at Oak Ridge National Laboratory \(NEWSWISE, 12/3\)](#)

Governor Phil Bredesen today joined officials from the University of Tennessee and the U. S. Department of Energy in dedicating a new state-funded research facility at Oak Ridge National Laboratory.

[ORNL's research reactor revamps veteran neutron scattering tool \(Lab Manager Magazine, 11/10, by Katie Freeman\)](#)

The Cold Triple Axis spectrometer, a new addition to ORNL's High Flux Isotope Reactor and a complementary tool to other neutron scattering instruments at ORNL, has entered its commissioning phase.

The most up-to-date news articles featuring neutron science performed at ORNL are available at <http://neutrons.ornl.gov/media/news/current-news.shtml>. You can sign up for an RSS feed [here](#) for ORNL Neutron Sciences. To receive ORNL news via twitter, use <http://twitter.com/oakridgelabnews>.