Oak Ridge National Laboratory
Neutron Sciences Progress Report
February 2010

Neutron Highlights

At HFIR, Cycle 426 ended January 30, 2010, and included 41 irradiation and 4 neutron activation analysis capsules. Cycle 427 began February 19, 2010, and is expected to end about March 14, 2010. Cycle 428 will begin May 5, 2010.

At SNS, neutron production ended December 22, 2009, and resumed February 22, 2010. External users will begin their visits during the first week of March 2010 and extending through June 29, 2010.

Call for proposals deadline is March 3, 2010, for the June–November 2010 period. See details.

This is the first announcement of a new **User Partnership Program for Sample Environment Equipment**. User ideas are needed for this collaborative activity.

Neutron & X-ray Scattering School deadline for applications is **March 8, 2010.**

Science Highlights

Neutron scattering experiments offer strong evidence that, if high-temperature superconductivity (HTSC) is related to a material's magnetic properties, the same mechanisms give rise to superconductivity in both copper-based (cuprate) and iron-based superconductors. The work, published in *Nature Physics*, was performed at SNS and HFIR and at the ISIS Facility in the United Kingdom. The ORNL researchers subjected single crystals of an iron, tellurium, and selenium material to neutron scattering analysis. HTSC research has centered around questions about the relationship between superconductivity and magnetic excitations. The results in this effort showed that the magnetic excitations in the iron-based material are described by the same wavelength and can be characterized by the same model as the excitations in superconducting cuprates. M. D. Lumsden, A. D. Christianson, E. A. Goremychkin, S. E. Nagler, H. A. Mook, M. B. Stone, D. L. Abernathy, T. Guidi, G. J. MacDougall, C. de la Cruz, A. S. Sefat, M. A. McGuire, B. C. Sales, and D. Mandrus. "Evolution of spin excitations into the superconducting state in FeTe1−xSex," *Nature Materials*, published online January 17, 2010.

The Workshop on the VULCAN Engineering Diffractometer was attended by more than 150 researchers in January 2010 to mark the completion of the VULCAN engineering diffractometer. The instrument received its first neutrons in June 2009. The workshop summarized the status of the research field and identified science problems on which VULCAN is expected to make an impact. Brainstorming sessions allowed participants to provide feedback on new capabilities needed for VULCAN, access to the instrument, and scientific and industrial uses. Details of the workshop are available.

Quasielastic neutron scattering (QENS) is the technique of choice for studying the mobility of ions in room temperature ionic liquids (RTILs), which are promising ionic charge-carrying media for advanced batteries and supercapacitors. Recent (2008–2009) experiments on BASIS, the backscattering spectrometer at SNS designed and built for QENS studies, have identified several distinct dynamic components in RTILs in bulk form. Under the umbrella of the Fluid Interface Reactions, Structures, and Transport EFRC at ORNL, the studies have been expanded to include RTILs confined in carbon-based nanomaterials, such as nano-onions,

and other porous media. The team includes D. Weslowski (ORNL), S. Dai (ORNL), Y. Gogotsi (Drexel University), and E. Mamontov (ORNL).

Researchers from GM (S. Jorgenson), Sandia Labs' Transportation Energy Center (D. Dedrick and T. Johnson), and ORNL (A. Payzant and J. Fernandez-Baca) are using HFIR's Wide-Angle Neutron Diffractometer to **characterize hydrogen content in tubes charged with sodium alanates**. This effort, which is also supported by the HTML User Program, will provide the first 3-dimensional map of hydrogen absorption in specific locations and how it changes as the tubes fill. Workable hydrogen storage is essential to transitioning to a hydrogen-based energy system. Results enabled the team to resolve C, NaH, NaCl, Na3AlH6, and Al phases in an uncharged tube and resolve alanate peaks in discharged and partially charged tubes. The data will elucidate mass transport mechanisms and determine the accuracy of mass transport models, which will enable optimization efforts. In situ absorption/ desorption experiments with deuterium will be conducted on VULCAN at SNS and the neutron imaging capability at HFIR. Solid-state hydrogen storage could improve energy density and increase the range of fuel cell vehicles by a factor of two compared with high-pressure hydrogen storage.

Instruments and Users

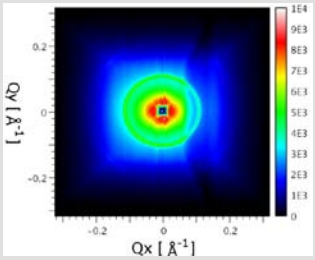
Call for proposals being accepted in the IPTS proposal system for the experimental period June through November 2010 (the call **deadline is March 3, 2010**). For more information please see our web site. More than 400 proposals were received during the last call.

We are pleased to announce a new **User Partnership Program for Sample Environment (SE) Equipment** to encourage collaborative development of SE equipment with users. Proposals for these limited funds will be developed with user teams, and then reviewed and prioritized by the Sample Environment Steering Committee (an existing group of internal and external scientists). Projects will be awarded and started as budget allows. Contact Lou Santodonato for details.

POWGEN (SNS BL-11A, Powder Diffractometer) is ready for commissioning and early user experiments.

HFIR Four-circle Diffractometer is open to users (HB-3A). This instrument is ideally suited for small unit-cell crystallography, particularly magnetic structures, and is equipped with a 4 K closed-cycle refrigerator. The current detector also has a continuous scan mode in addition to the traditional step scanning mode, greatly increasing the data collection rate. A tunable horizontal bending of the monochromator significantly enhances the scattered intensity from the sample. Either high resolution or high intensity modes are available. Crystal samples typically around 3 mm^3 or larger are suitable, and wavelengths of 1.0 or 1.5 Å are available.

The commissioning of **EQ-SANS** (SNS, BL-6) is well under way. Preliminary measurements indicate that the instrument has met its major design specifications of wide Q-coverage, high intensity, and good wavelength resolution. Its innovative frame-skipping operation allows it to cover two decades in Q-range with one experimental setting (e.g., 0.003–0.4$Å^{-1}$). The counting statistics are extremely good. Absolute flux measurement is planned. A 45-cell automated sample exchanger with temperature control (–20 to 80°C) is being tested and will be ready for users soon. The figure below shows TOF-scattering data of a silver behenate sample reduced to intensity vs. (Q_x, Q_y). If you are interested in becoming a user during the commissioning stage of EQ-SANS, please contact J.K. Zhao, zhaoj@ornl.gov



The TOPAZ detector frame was recently installed (SNS BL-12, Single Crystal Diffractometer, see image below). It is beginning its commissioning.

The **Nanoscale Ordered Materials Diffractometer** (NOMAD, SNS BL-1B) will begin commissioning in summer 2010. See the progress below. NOMAD is a high-flux, medium-resolution diffractometer for SNS using a large bandwidth of neutron energies and extensive detector coverage to carry out structural determinations of local order in crystalline and amorphous materials.

The **neutron guide for MaNDi** (SNS, BL-11B, Macromolecular Neutron Diffractometer) was recently installed (see image below). Instrument commissioning will begin in 2013.

The optics concept has been developed for **IMAGINE** (HFIR, CG-4A). Procurements for the diffractometer and the optics are under way. Commissioning will begin during summer 2011. **IMAGINE** is a state-of-the-art neutron image-plate single-crystal diffractometer at HFIR

VISION (Vibrational Spectrometer, SNS, BL-16B) is under construction (image below). Upon completion by the end of 2011, VISION will be among the best instruments in its class. The advanced neutron optical concept features neutron guides with coatings up to m=7, large-area crystals analyzer modules with spatial and time focusing, and high-flux medium-resolution powder diffraction capabilities.

.

The **HYSPEC** (Hybrid Spectrometer, SNS BL-14B) beam line currently has the mounting base for the T0 Chopper and the housing for the T1A Disk Chopper installed and the beam guide installation (see image below) is complete to 24 m. The HYSPEC external building was completed in December 2009.

New 'End of Experiment' report requirement: Beginning with the current experimental cycle (December 2009 - May 2010), 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.

Publication citations are needed for reports to our sponsor. Please use the acknowledgment for HFIR or SNS experiments; complete the form or send the citation to neutronusers@ornl.gov.

The **cafeteria** in the SNS Central Lab and Office building opened January 4, 2010. Hours are 7–9:30 a.m. for breakfast and 10:45 a.m.–1:15 p.m. for lunch.

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 travels to discuss experiments before and after the measurements. Contact Hope Moore-Webb for details.

The **SNS schedule** in the coming months may be perturbed by the planned, but undetermined, end of life of the mercury target. This foreseen operational event will cause the shutdown of SNS for about two weeks while a new target is installed. Users will be notified as soon as possible and rescheduled to a future time. Our goal is to predict the target end of life and schedule future target replacements within normal maintenance periods.

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.”

- Powder Diffraction Group Leader (NC50209258)
- Senior Scientist – Energy Materials (NC50209243)

- Senior Scientist – Environmental Geosciences (NC50209243)
- Senior Scientist – Nano-structured Materials (NC50209243)
- Senior Scientist – Biological Systems (NC50209243)
- Neutron Scattering Science User Proposal Management Lead (NC50202940)
- EQ-SANS Instrument Scientist (NC50198520)
- Scientific Computing Scientist for SANS and Reflectometry (NC50205732)
- Accelerator Operations Manager (NC50206418)
- Collaborative Research Visits Program, including Visiting Student Thesis Research, Visiting Postdoctoral Research, and Faculty Research Sabbaticals; see http://neutrons.ornl.gov/crv/.

Neutron Sciences Career Development Program (http://www.orau.org/ornl/neutrons/) was founded to nurture the creative development of neutron scattering science and instrumentation at ORNL. This initiative is viewed as a critical part of keeping the neutron scattering instruments at ORNL on the cutting edge of design and scientific functionality, keeping them competitive worldwide. It is designed to provide an environment in which early-career scientists and technicians can be a part of innovative concepts for neutron-related research and instrumentation while helping end users develop proposals, conduct experiments, and analyze data. See opportunities for Neutron Scattering Instrument Scientist, Neutron Scattering Instrument Associate, and Neutron Scattering Technician.

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

- Postdoctoral Research Associate in Li-Based Battery Materials (ORNL10-73-NSSD)
- Data Acquisition Instrument Associate (ORNL10-62-NSSD)
- Postmaster's Research Associate for Nuclear Analyst/Physicist (ORNL10-50-NFDD)
- Postdoctoral Research Program in Neutron Scattering (ORNL10-39-NSSD)
- Postdoctoral Research Associate in Neutron Scattering (ORNL10-34-NSSD)
- Postdoctoral Research Associate in Neutron Scattering: thermoelectric materials (ORNL10-21-NSSD)
- Postdoctoral Research Associate for Developing the Spin-Echo Grazing Incidence Scattering (SERGIS) (ORNL10-17-NFDD)
- Postdoctoral Research Associate in Neutron Scattering: Organic superconductors (ORNL10-16-NSSD)
- Postdoctoral Research Associate in In-situ Neutron Scattering Studies of Fuel Cell Materials (ORNL10-06-NSSD)
- Postdoctoral Research Associates in SANS and Neutron Reflectometry Data Reduction and Analysis (ORNL10-02-NSSD)

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.orau.gov/orise/edu/ornl/. **Applications are open now.**

Meetings and Other Events of Interest to SNS and HFIR Users

March 15–19, 2010, American Physical Society Meeting, Portland, Oregon, USA. Visit the ORNL booth at #720.

March 19–20, 2010, Southeast Regional Collaborative Access Team (SER-CAT) Symposium and Board Meeting, Oak Ridge, Tennessee, USA.

April 20–21, 2010, Hydrogen and Helium Isotopes in Materials Conference, Oak Ridge, Tennessee, USA.

June 12–26, 2010, National School on Neutron and X-Ray Scattering, Argonne and Oak Ridge. Registration deadline is March 8, 2010.

June 13–18, 2010. 20th Annual VM Goldschmidt Conference, Knoxville, Tennessee, USA. This is the foremost meeting of the year for the worldwide geochemistry community.

June 26–30, 2010. American Conference on Neutron Scattering, Ottawa, Ontario, Canada.

July 24-29, 2010. American Crystallographic Association, Chicago, Illinois.

Proposal Call Dates for HFIR and SNS
March 3, 2010, midnight, Wednesday: proposals for the period June–November 2010
September 1, 2010, midnight, Wednesday: proposals for the period December 2010–May 2011
March 2, 2011, midnight, Wednesday: proposals for the period June–November 2011
September 14, 2011, midnight, Wednesday: proposals for the period December 2011–May 2012

Neutron Science in the News

Recent articles about the Oak Ridge neutron scattering program have appeared in **Neutron News** (v.21, issue 1).

Making Use Of Neutrons—Subatomic particles provide new ways to study structure, dynamics of materials; by Jyllian N. Kemsley (*Chemical and Engineering News*, 2/22/2010) Neutrons have some unsung properties that make them useful for investigating matter. Because they are neutral, they can penetrate deeper into a sample than electrons can. Because they have mass and spin, they have a magnetic moment and can probe magnetism.

Dr. Ian Anderson has explaining ORNL down to a science (WBIR, 2/9)
Dr. Ian Anderson is the Associate Laboratory Director for the Spallation Neutron Source at ORNL. He will bring to "Live at Five at Four" viewers a look at the amazing work being done in the science field right in our own backyard. He started with what SNS does.

Magnetism seen as key to superconductivity (EE Times 2/4)
Oak Ridge National Laboratory researchers are citing evidence that high-temperature superconductivity derives from the same mechanisms regardless of materials. That finding has prompted speculation that magnetic spin excitations that couple electrons are the key ingredient for superconductivity. Magnetic interactions "provide the glue that binds the electrons together," said Oak Ridge lead researcher Mark Lumsden. "The pairing up of electrons is essential for the formation of the macroscopic quantum state giving rise to superconductivity." High-temperature superconductivity could result in ultra-fast electronic devices that capitalize on high-speed electrons traveling in a material whose resistance has been reduced to zero. Levitating trains, ultra-sensitive sensors called superconducting quantum interference devices, and nuclear magnetic resonance imaging use superconductors. Using the Spallation Neutron Source and the High Flux Isotope Reactor, the researchers applied intense neutron beams to image single crystals of superconducting iron, tellurium, and selenium materials. They also observed the same spin excitations that are believed to be the source of superconducting in copper-based materials called cuprates.

Energy Grants Seek Reliable Source for Diagnostic Aid (N.Y. Times 1/26)
Amid a global shortage of a radioactive isotope used to diagnose cancer, heart disease, and kidney problems, the Energy Department on Monday moved to develop two radically different sources for the material. Supplies have been short since last May, when the reactor in Chalk River, Ontario, that used to be the biggest supplier of the isotope was shut down because of a leak. … Primarily a research reactor, the High Flux Reactor at the Oak Ridge National Laboratory also produces medical isotopes.

VULCAN workshop at Spallation Neutron Source (Knoxville News Sentinel 1/20)
VULCAN, one of the new research instruments at the Spallation Neutron Source, will be the topic of a workshop Thursday and Friday at Oak Ridge National Laboratory. The engineering diffractometer received its first neutrons back in June and, according to ORNL neutron chief Ian Anderson, the Canadian-sponsored instrument is expected to become a staple of industrial research for years to come. Anderson said VULCAN was funded by the Canada Foundation for Innovation and, as such, Canada gets access to 20 percent of the beam time on the instruments (or the equivalent on other instruments). "It's one of the instruments where we expect to get a lot of interest from industry to use it," he said.

The most up-to-date news articles featuring neutron science performed at ORNL are available at http://neutrons.ornl.gov/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.