

The banner features a blue background with a molecular lattice structure on the right and a blurred image of a person's face on the left. The text is in white and yellow.

Oak Ridge National Laboratory Neutron Sciences Progress Report October 2010

Neutron Highlights

The next [call](#) for HFIR and SNS proposals deadline is **March 2, 2011**, for the June–November 2011 period.

At HFIR, Cycle 431 began October 13, 2010, and will end November 5, 2010. The HFIR long-term schedule is [available](#).

At SNS, the current cycle of neutron production began August 25, 2010, and will end December 20, 2010. The detailed SNS schedule is [available](#). Recent availability is approaching 95%.

User numbers are growing. For the year October 2009–September 2010, HFIR had 375 unique users (compared with 358 the previous year) and SNS had 422 unique users (307 in the previous year). A unique user is one who visited the facility to perform a peer-reviewed experiment at least once during this period.

Presentations from [ORNL User Week](#), September 13–17, 2010, including the [Workshop on Neutrons for Catalysis](#) are available from the websites.

Science Highlights

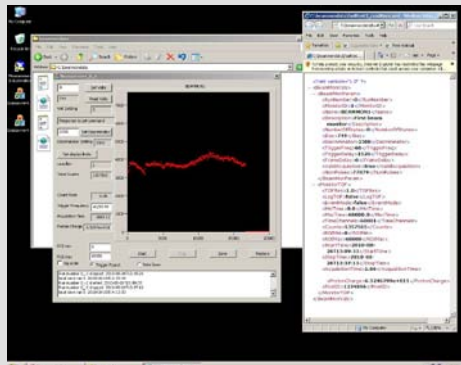
Inelastic neutron experiments were conducted at the Wide Angular-Range Chopper Spectrometer (ARCS at Spallation Neutron Source) and the HB-3 triple-axis spectrometer (High Flux Isotope Reactor) instruments on superconducting $\text{Ba}(\text{Fe}_{0.926}\text{Co}_{0.074})_2\text{As}_2$. The collective magnetic excitations were observed close to the magnetic ordering vector of the parent BaFe_2As_2 compound. At low energies, the excitations have a pronounced in-plane anisotropy that can be associated with frustrated versus *satisfied* nearest neighbor interactions in the parameter regime of dynamic nematic correlations. The spin resonance in the superconducting state is found to have the same anisotropy. At energies above 80 meV, quasipropagating modes are observed experimentally along the transverse direction while modes in the LO direction appear to have a very large energy scale. This was presented as a Rapid Communication and Editor's Suggestion in *Physical Review B*. H.-F. Li, C. Broholm, D. Vaknin, R. M. Fernandes, D. L. Abernathy, M. B. Stone, D. K. Pratt, W. Tian, Y. Qiu, N. Ni, S. O. Diallo, J. L. Zarestky, S. L. Bud'ko, P. C. Canfield, and R. J. McQueeney, "Anisotropic and quasipropagating spin excitations in superconducting $\text{Ba}(\text{Fe}_{0.926}\text{Co}_{0.074})_2\text{As}_2$," *Phys. Rev. B* **82**, 140503 (2010).

Multiferroic materials, which exhibit both magnetic and ferroelectric order, could enable the use of electrical fields to control magnetic polarization and vice versa. They have great potential for applications such as advanced electronics and sensors. Multiferrocity was recently found in frustrated magnets; determining the underlying magnetic ground state for the materials is critical to a complete understanding of the phenomenon. The triangle lattice CuFeO_2 exhibits magnetic frustration within each hexagonal plane. A multiferroic phase can be induced either by applying a magnetic field above 7 T or by doping with nonmagnetic Al or Ga impurities. Neutron scattering at the HFIR Triple Axis HB-1 and the SNS Cold Neutron Chopper Spectrometer, combined with theoretical modeling, showed lattice distortions are important in determining the magnetic ground state of Ga-doped CuFeO_2 . The complex ground state provides an alternative way to realize multiferroic coupling, whereby displacements of the oxygen atoms severely distort the spin configuration and produce the electric polarization. The predicted and observed dynamical fingerprints of the multiferroic phase were in close agreement. Many other frustrated magnets with rhombohedral or hexagonal symmetries may exhibit the same form of multiferroic coupling as doped CuFeO_2 . The symmetry of these materials makes them excellent candidates for exotic magnetoelectric control. J. T. Haraldsen, F. Ye, R. S. Fishman, J. A. Fernandez-Baca, Y. Yamaguchi, K. Kimura, and T. Kimura, "Multiferroic phase of doped delafossite CuFeO_2 identified using inelastic neutron scattering," *Physical Review B* **82**, 020404 (2010).

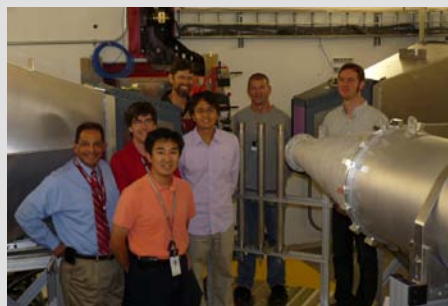
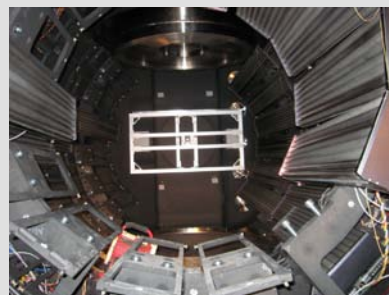
Three publications reporting results from ORNL neutron sources during the last three years have been cited more than 100 times:

- C. de la Cruz, et al., "Magnetic order close to superconductivity in the iron-based layered $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$ systems," *Nature* **453**, 899–902(2008). **560 citations**. Performed at HFIR HB1A and NIST.
- J. Zhao, et al., "Structural and magnetic phase diagram of $\text{CeFeAsO}_{1-x}\text{F}_x$ and its relation to high-temperature superconductivity," *Nature Materials*, **7**(12): 953-959(DEC 2008) **188 citations**. Performed at HFIR HB3.
- M. A. McGuire, et al., "Phase transitions in LaFeAsO : Structural, magnetic, elastic, and transport properties, heat capacity and Mossbauer spectra," *Physical Review B* **78**(9), 094517(SEP 2008). **108 citations**. Performed at HFIR HB1A, WAND and HB3.

New or Expanded Capabilities

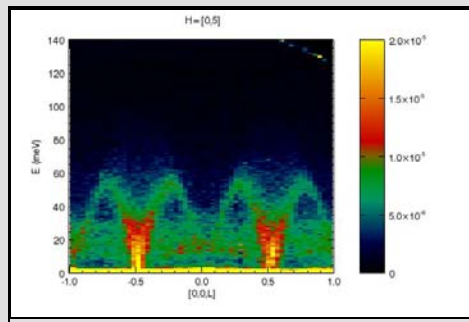


NOMAD (SNS BL-1B) began commissioning in August 2010. The image (left) is the first neutron spectrum recorded at the beam monitor position. The detector tank is pictured to the right. NOMAD will enable studies of a large variety of samples, ranging from liquids and solutions, glasses, and nanocrystalline materials to long-range-ordered crystals. It will use a large bandwidth of neutron energies and extensive detector coverage to carry out structural determinations of local order in crystalline and amorphous materials.



VULCAN helps users from GM and Sandia National Laboratory develop hydrogen storage materials for next-generation fuel cell cars. Left to right: Edgar Lara-Curzio and Andrew Payzant of ORNL's High Temperature Materials Laboratory, Xun-Li Wang, Scott Jorgensen of GM, Ke An, Terry Johnson of Sandia, and Harley Skorpenske. The team uses VULCAN to map hydride distribution in fuel cell tubes (three mounted on the instrument).

ORNL staff H. Bilheux and B. Hill of Neutron Sciences, A. Vass of Biological Sciences, T. Nichols of Measurement Science and Systems Engineering, and colleagues from the University of Tennessee College of Veterinary Medicine, Small Animal Clinic Sciences, and Department of Oncology are joining forces to investigate a novel approach to forensic analysis using neutron imaging techniques. Structural changes in a broad selection of tissue samples will be studied using neutron imaging as a method to estimate the time of death. This research is sponsored by the Department of Justice, National Institute of Justice, Office of Investigative and Forensic Sciences.



An example measurement of the spinon spectrum in a single crystal sample of KCuF_3 is shown above.

SEQUOIA, the Fine Resolution Fermi Chopper Spectrometer at SNS BL-17, has completed a recently initiated extended commissioning program. We are engaging the user community of newly completed instruments to assure an instrument is ready for experimental use. This means it can acquire the necessary data, with standard sample environment, and that data can be reduced and analyzed for publication. The SEQUOIA instrument team, led by [Garrett Granroth](#), in collaboration with several users, carried out tests and experiments to assess and improve the science readiness. Graduate students assisted in these tests to enhance their knowledge of the instrument commissioning process. Several results from these experiments have been submitted for publication. Other instruments in this program at SNS are VULCAN, TOPAZ, POWGEN, EQ-SANS, and NOMAD. At HFIR, the U.S. Japan Cold Triple-Axis Spectrometer will begin commissioning shortly. We want your engagement in this process for these and future instruments.

The “FERNS” (Fast Exchange Refrigerator for Neutron Science) has been commissioned for user experiments on the POWGEN powder diffractometer. It features a remote sample changer of 24 samples.

A total of 67 students participated in summer internships at HFIR and SNS; this is almost double the total in the previous year. Some were advanced high school students and some were teachers doing research over the summer to take back to their high school classes. Colleges and universities represented by the students and visiting faculty included Pellissippi State Technical Community College, Southern Illinois University, Western Kentucky University, Virginia Polytechnic Institute, University of Michigan, Whitworth College, the University of Tennessee at Knoxville and Chattanooga, Georgia Tech, University of Cincinnati, Oregon State University, Tennessee Technical University, East Tennessee State University, Hope College, Middle Tennessee State University, Rhodes College, University of Northern Texas, University of Wisconsin–Madison, Harvard, and Yale.

Brief Items about Instruments, People, and Users

More than 640 proposals were received for the [call for proposals](#) that closed August 25, 2010, for beam time at 22 instruments (10 at HFIR and 12 at SNS). The Science Review Committees meet October 18–19, 2010, to rank the proposals.

Yang Zhang has been named a Shull Fellow. He came to ORNL from MIT where he finished his Ph.D. in Nuclear Science and Technology in August 2010. He will investigate the physics of fluids, glasses, and soft materials using neutron scattering and high-performance computing simulation at ORNL.

University of Tennessee and ORNL scientists are moving into the **Joint Institute for Neutron Sciences**. A formal ribbon cutting will be held soon at this building located adjacent to SNS and the Center for Nanophase Materials Sciences.

Peer-reviewed publications so far identified for calendar year 2009 total 197 by SNS staff or using SNS resources, and 155 for HFIR staff or resources. There is some duplication among the two groups.

Publication citations are needed for reports to our sponsor and for selection of annual report highlights.

Please send the citation to neutronusers@ornl.gov if your publication is not included on our [lists](#). There is a standard [acknowledgment](#) for HFIR or SNS experiments.

DOE’s Basic Energy Sciences Advisory Committee issued a [report](#) on **Science for Energy Technology: Strengthening the Link between Basic Research and Industry**. It summarizes the results of a Workshop on Science for Energy Technology on January 18–21, 2010, to identify the scientific priority research directions needed to address the roadblocks and accelerate the innovation of clean energy technologies. Chapter 11 focuses on the role of user facilities.

The **2011 U.S. National School on Neutron and X-ray Scattering** is tentatively scheduled for June 12–18, 2011 in Oak Ridge and June 18–25, 2011, at Argonne. More information and application details will be available later this year 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](#) for the 2010 NXS School.

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 travels to discuss experiments before and after the measurements. Contact [Hope Moore-Webb](#) for details.

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)

- Powder Diffraction Group Leader (NC50235310)
- Neutron Sciences Industrial Liaison (NC50235889)
- Scientific Data Analysis Group Leader (NC50233131)
- Target Systems Group Leader (NC50229927)
- Instrument Development Leader (NC50232757)
- 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

- [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)
- [Neutron Scattering Instrument Scientist in Neutron and/or X-ray Diffraction](#) (ORNL10-128-NSSD)
- [Postgraduate Instrument Associate](#) (ORNL10-114-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.ornl.gov/orise/edu/ornl/>.

Applications are open now.

Meetings and Other Events of Interest to SNS and HFIR Users

October 31–November 3, 2010. [Neutrons and Food*](#), Sydney, Australia

November 30–December 4, 2010. [2010 American Chemical Society 66th Southwest / 62nd Southeast Regional Meeting](#), New Orleans, LA. ORNL is participating in the exhibit and graduate fair.

February 17–21, 2011. [2011 American Association for the Advancement of Science Annual Meeting](#), Washington, D.C. ORNL is participating with a booth.

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

*One potential outcome of these events is a book in the series Neutron Scattering Applications and Techniques. Volunteers are needed to develop additional topics in this series; support may be available. Contact Al Ekkebus, ekkebusae@ornl.gov, for more information.

Future proposal call dates for HFIR and SNS

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

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

Neutron Science in the News

[Brookhaven research instrument gets new life at Oak Ridge reactor \(Knoxville News Sentinel, 10/10\)](#) A new research instrument is being commissioned at Oak Ridge National Laboratory's High Flux Isotope Reactor. According to info from ORNL, the cold triple-axis spectrometer was originally at Brookhaven National Lab's High Flux Beam Reactor and was then moved to Oak Ridge and refurbished for use at the HFIR.

Tennessee's science enterprise aims to capitalize on institutional strengths, a government lab, and low costs of living.

(Nature Jobs) The research focus of Oak Ridge National Laboratory has shifted [since the Manhattan Project] from weapons development to a variety of other energy-related topics. Interview with Thom Mason.

Scientific upgrades at the High Flux Isotope Reactor at Oak Ridge National Laboratory. "Cold" neutron beam lines have been added, broadening the HFIR's range as an experimental and testing facility, by Douglas L. Selby and Gregory S. Smith, *Nuclear News*, September 2010, cover article, pp 35–41.

Academies Creating Teacher-Scientists Professional Development Program (ACTS). Through ACTS, 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 the Lab and with their students back home. Elaine Custer—a physics, math, and computational sciences teacher from Karns City, Pennsylvania —just finished her second year working with scientists at the SNS TOPAZ instrument.

Neutrons helping ORNL researchers unlock secrets to cheaper ethanol (domain-b.com, 21 September 2010). Researchers from the Department of Energy's Oak Ridge National Laboratory and Georgia Tech used small-angle neutron scattering to probe the structural impact of an acid pretreatment of lignocellulose from switchgrass. Pre-treatment is an essential step to extract cellulose, which can through a series of enzymatic procedures be converted into sugars and then ethanol.

'User Week' at ORNL (*Knoxville News Sentinel*, September 13, 2010). Oak Ridge National Laboratory is staging a five-day workshop this week for potential researchers at its national user facilities, with about 200 visiting researchers participating in the event, according to lab info. The purpose is to highlight opportunities for collaboration with lab researchers in unique facilities such as the Center for Nanophase Materials Sciences, High Flux Isotope Reactor, High Temperature Materials Laboratory, National Center for Computational Sciences, and Spallation neutron Source.

Consortium of Tennessee universities receive \$20 million grant (Chattanooga.com, September 10, 2010). Governor Phil Bredesen joined a consortium of public and private universities in the state on Thursday to announce a \$20 million grant from the National Science Foundation (NSF) to boost the state's energy-related research and education efforts. The grant is one of the largest ever awarded in Tennessee by the NSF. A coalition of scientists, faculty and students from 11 public and private universities in Tennessee and Oak Ridge National Laboratory (ORNL) will be grouped together into "network nodes" for conducting research, mentorship and outreach.

Dr. Know (WBIR, 8/17/2010). Dr. Ian Anderson from ORNL talks about the student scientists.

Dr. Know (WBIR, 10/10/2010). Dr. Ian Anderson from ORNL talks about making medicine work for you.

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>.