SHUG (SNS HFIR User Group), http://neutrons.ornl.gov/users/shug/
SHUG executive committee minutes.
Teleconference held September 21, 2010.
Attendees:

Executive Committee: Cora Lind, Matthew Stone, Peter Khalifah, Mike Crawford, Antonella Longo, Greg Beaucage, Pat Woodward.

Guests: Al Ekkebus, Greg Smith (Group leader for the Low-Q group)

Minutes submitted for review October 20, 2010 by M. B. Stone.

ACTION ITEMS:
Next telecom Tues Oct 12
If you have a paragraph to send to Al regarding proposed neutron scattering workshops, please do so.

ATTACHMENTS and WEBSITES of interest from the teleconference:

Handouts that were distributed to attendees of the Neutrons for Catalysis Workshop.

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1. Report on User Week and Neutrons for Catalysis (Cora, Peter, Al)

The basic science session was held on Monday with approximately 100 attendees. The capabilities and facilities at ORNL were discussed. There were tours available of the SNS facility. The session on Tuesday with approximately 100 attendees was focused upon applied sciences, including a discussion of how industry interacts with ORNL. The Nano-center user meeting was held on Tuesday. The Nano-center had further sessions the rest of the week.

The neutrons for catalysis workshop was held Thursday and Friday. There were a series of talks both from the neutron user community and outside the neutron community. There were representatives from industry, national laboratories, and universities. There were excellent break-out sessions for exchanging ideas between these communities. There were encouraging remarks that additional workshops should be done in the future, especially with the construction of the guest house, to have additional interaction with the ORNL scientists.

One idea which was discussed with Cora was to create a centralized web-based ‘drop-box’ or ‘request box’ which would give novices a way to present an idea for an experiment and allow the people at ORNL to distribute these questions to the appropriate scientists and beam-line scientists for further discussion and evaluation. Argonne has a link on their web-page for asking general questions of scientists (http://www.newton.dep.anl.gov/aasquesv.htm). Something similar could be done for potential users.

2. Potential programs for next year's User Week

Data reduction and analysis workshop for inelastic scattering. Diffraction is very often taught, but inelastic scattering is rarely taught in-depth. A potential component of this would be to set aside time to do a very brief experiment using an inelastic instrument, or have a more detailed tour of the inelastic suite.

Any workshop should also include the instrument scientists for discussion of measurement capabilities, how to write good proposals for neutron experiments, and a tour of the instrument (hopefully when the facility is operating) to see an experiment in progress.

Additional ideas for future user weeks at ORNL: on-site synthesis and on-site characterization, nano-materials, specialized (not just extreme) sample environments (sheer cells, low-background, high-temperature, pressure, low-temperature, magnetic field). There could be a separate workshop just for sample environments.

3. Other outreach ideas?

4. News at ORNL (Greg Smith- Group leader for the Low-Q group)

There were 420 proposals for SNS, and 224 for HFIR submitted. This is an increase of 25% at SNS and 5% at HFIR. This follows the increase in instruments available at the facilities. The scientific review committees will meet on October 18 and 19. Notifications are being planned to be sent out on the week of the 25th of October.

There was oil contamination in the cryogenic moderator at SNS at the start of the cycle. It is running at 780 or 750 kW currently.

HFIR finished 7 full reactor cycles this fiscal year

The CTAX (cold triple-axis) will start experimental commissioning in mid-October.

The imaging beamline at HFIR has entered the user program on a part-time basis.

POWGEN currently has 10% detector area coverage with 10% more coverage to be installed at the end of 2010, and 10% more to be installed at the end of Feb 2011. The ghosting issue associated with the original POWGEN and VULCAN detectors has been improved by addressing both hardware changes and software compensation

NOMAD at SNS has completed CD4 and is now commissioning with beam.

The JINS building is open and people are moving in.

The guesthouse will be finished with external construction by the end of 2010, with internal work proceeding through beginning of 2011.

NoBugs meeting is in mid October.

5. The SHUG Executive Committees concerns regarding POWGEN.

The SHUG executive committee discussed that there are still issues beyond detector ghosting regarding the POWGEN instrument. These concerns are based upon both direct experience using the POWGEN instrument as well as formal discussions with the instrument team.

The two major concerns are detector efficiency and background.

1) Detector efficiency is very low and improving detector electronics and other hardware will be necessary to bring Powgen to its full potential. It would be beneficial for the user community if dedicated resources (work time allocation of electronics specialists, testing time for detectors) could be allocated to make every possible effort to improve detector efficiency.

2) There are concerns with sample dependent background. Some samples work very well, others yield extremely poor signal to noise suggesting up to 70% incoherent contribution. These large incoherent signals are not appropriate given the composition of the materials being examined.

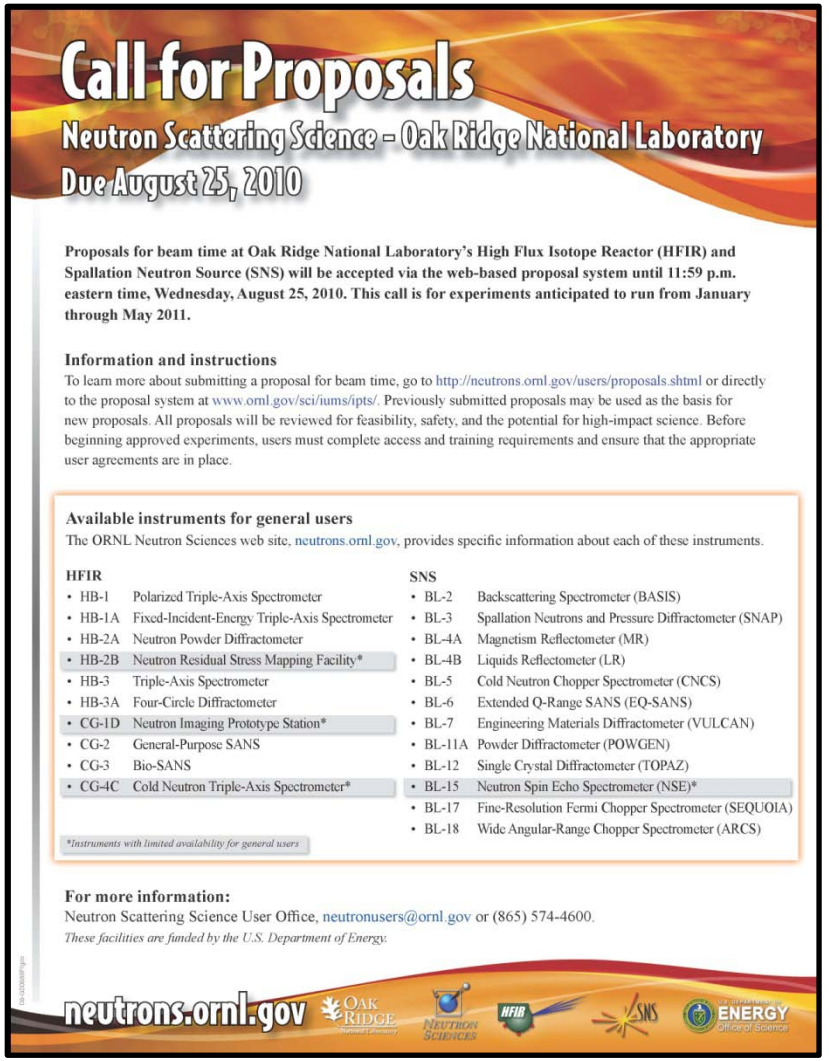
On behalf of the SHUG executive committee and for the benefit of the powder diffraction community, it is crucial that the instrument scientists be given appropriate time to work on understanding these issues to make appropriate recommendations for a solution. We also encourage further testing, research and development on behalf of the detector group to understand and improve the efficiency of the POWGEN and VULCAN detectors.

Collaborating with ORNL's Neutron Scattering Facilities HFIR and SNS

- Become a user
- Collaborative Research Visits – Sabbatical & Visitor program
  - http://neutrons.ornl.gov/crv/application.shtml
- User Partnership Program for Sample Environment Equipment Development
  - http://neutrons.ornl.gov/instruments/SNS/sample/
- Promote ORISE internships, fellowships, and research participation programs
  - http://orise.orau.gov/sep/index.htm
- Travel grants for faculty and students from EPSCoR institutions
- ORNL jobs and ORAU positions

Become a User

- Open access based on scientific quality
- Apply for beam time though competitive proposal process
  - Submit proposal using on-line system
    - 2-page statement of research plus sample description
    - 2 calls per year
  - External peer review required
  - Must be technically feasible and safe
- Free of charge if experimental results published
- Proprietary users (results are not shared) are charged to recover costs



Call for Proposals

Neutron Scattering Science – Oak Ridge National Laboratory

Due August 25, 2010

Proposals for beam time at Oak Ridge National Laboratory's High Flux Isotope Reactor (HFIR) and Spallation Neutron Source (SNS) will be accepted via the web-based proposal system until 11:59 p.m. eastern time, Wednesday, August 25, 2010. This call is for experiments anticipated to run from January through May 2011.

Information and instructions

To learn more about submitting a proposal for beam time, go to http://neutrons.ornl.gov/users/proposals.shtml or directly to the proposal system at www.ornl.gov/sci/iums/ipts/. Previously submitted proposals may be used as the basis for new proposals. All proposals will be reviewed for feasibility, safety, and the potential for high-impact science. Before beginning approved experiments, users must complete access and training requirements and ensure that the appropriate user agreements are in place.

Available instruments for general users

The ORNL Neutron Sciences web site, neutrons.ornl.gov, provides specific information about each of these instruments.

HFIR		SNS	
• HB-1	Polarized Triple-Axis Spectrometer	• BL-2	Backscattering Spectrometer (BASIS)
• HB-1A	Fixed-Incident-Energy Triple-Axis Spectrometer	• BL-3	Spallation Neutrons and Pressure Diffractometer (SNAP)
• HB-2A	Neutron Powder Diffractometer	• BL-4A	Magnetism Reflectometer (MR)
• HB-2B	Neutron Residual Stress Mapping Facility*	• BL-4B	Liquids Reflectometer (LR)
• HB-3	Triple-Axis Spectrometer	• BL-5	Cold Neutron Chopper Spectrometer (CNCS)
• HB-3A	Four-Circle Diffractometer	• BL-6	Extended Q-Range SANS (EQ-SANS)
• CG-1D	Neutron Imaging Prototype Station*	• BL-7	Engineering Materials Diffractometer (VULCAN)
• CG-2	General-Purpose SANS	• BL-11A	Powder Diffractometer (POWGEN)
• CG-3	Bio-SANS	• BL-12	Single Crystal Diffractometer (TOPAZ)
• CG-4C	Cold Neutron Triple-Axis Spectrometer*	• BL-15	Neutron Spin Echo Spectrometer (NSE)*
		• BL-17	Fine-Resolution Fermi Chopper Spectrometer (SEQUOIA)
		• BL-18	Wide Angular-Range Chopper Spectrometer (ARCS)

*Instruments with limited availability for general users

For more information:

Neutron Scattering Science User Office, neutronusers@ornl.gov or (865) 574-4600.

These facilities are funded by the U.S. Department of Energy.

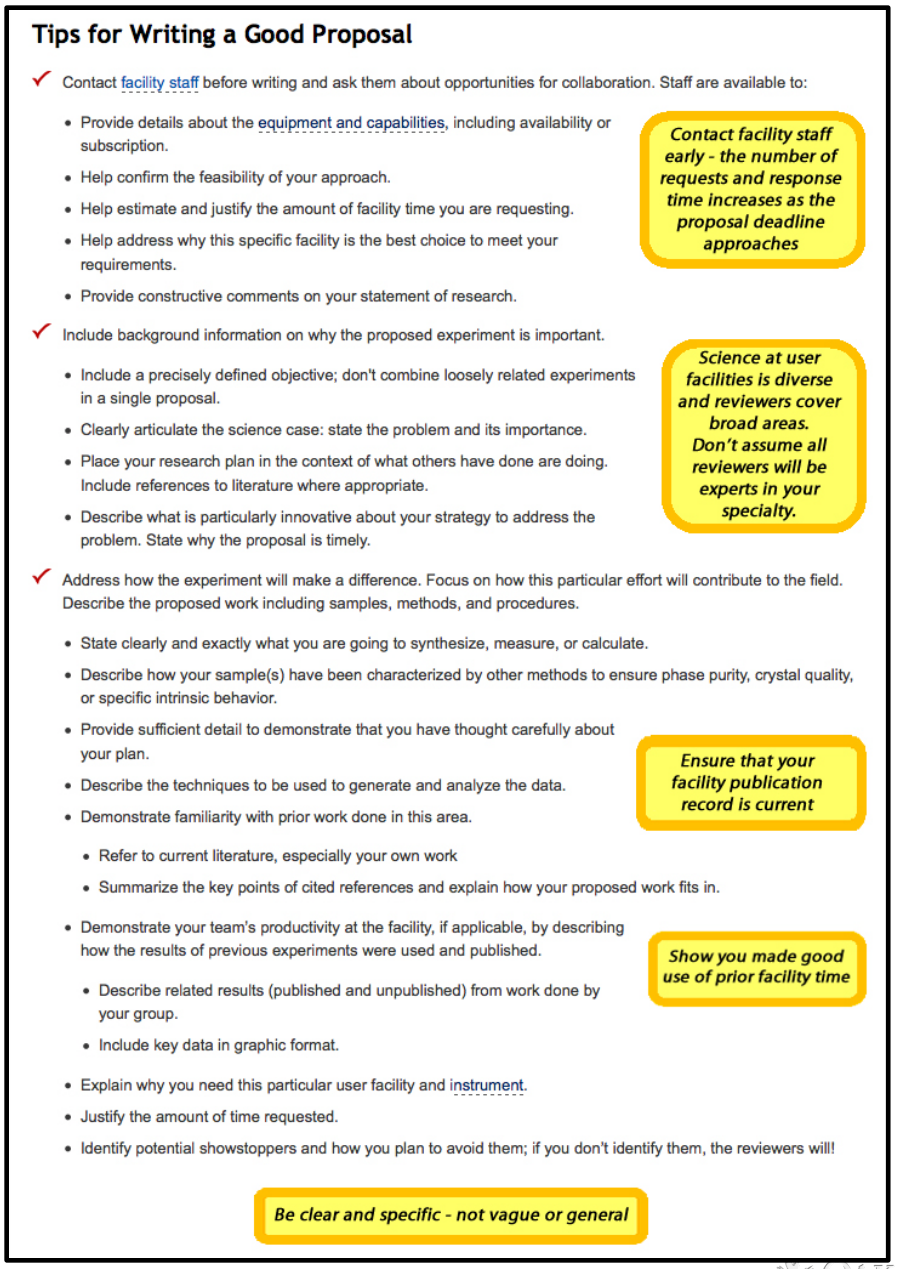
neutrons.ornl.gov

First-time Users Get Started with Our Assistance

- Contact an Instrument Scientist to discuss your research
  - What is the research problem
  - How mature is the research project
  - What is the material – composition, form, size, availability
  - What are the experimental conditions (temperature, pressure, magnetic field, etc)
  - What will be measured
  - How will results be presented and to whom
- TEST TIME – proof of principal, rapid access – contact Inst. Scienist.

Proposal Tips

- Developed using our Reviewers' feedback
- Reviewed by User Groups
- Posted on our Web Site: http://neutrons.ornl.gov/users/proposal-tips.shtml
- Referenced and linked in the proposal Statement of Research template



Tips for Writing a Good Proposal

✓ Contact facility staff before writing and ask them about opportunities for collaboration. Staff are available to:

- Provide details about the equipment and capabilities, including availability or subscription.
- Help confirm the feasibility of your approach.
- Help estimate and justify the amount of facility time you are requesting.
- Help address why this specific facility is the best choice to meet your requirements.
- Provide constructive comments on your statement of research.

Contact facility staff early - the number of requests and response time increases as the proposal deadline approaches

✓ Include background information on why the proposed experiment is important.

- Include a precisely defined objective; don't combine loosely related experiments in a single proposal.
- Clearly articulate the science case: state the problem and its importance.
- Place your research plan in the context of what others have done are doing. Include references to literature where appropriate.
- Describe what is particularly innovative about your strategy to address the problem. State why the proposal is timely.

Science at user facilities is diverse and reviewers cover broad areas. Don't assume all reviewers will be experts in your specialty.

✓ Address how the experiment will make a difference. Focus on how this particular effort will contribute to the field. Describe the proposed work including samples, methods, and procedures.

- State clearly and exactly what you are going to synthesize, measure, or calculate.
- Describe how your sample(s) have been characterized by other methods to ensure phase purity, crystal quality, or specific intrinsic behavior.
- Provide sufficient detail to demonstrate that you have thought carefully about your plan.
- Describe the techniques to be used to generate and analyze the data.
- Demonstrate familiarity with prior work done in this area.
  - Refer to current literature, especially your own work
  - Summarize the key points of cited references and explain how your proposed work fits in.
- Demonstrate your team's productivity at the facility, if applicable, by describing how the results of previous experiments were used and published.
  - Describe related results (published and unpublished) from work done by your group.
  - Include key data in graphic format.
- Explain why you need this particular user facility and instrument.
- Justify the amount of time requested.
- Identify potential showstoppers and how you plan to avoid them; if you don't identify them, the reviewers will!

Ensure that your facility publication record is current

Show you made good use of prior facility time

Be clear and specific - not vague or general

For More Information

- Visit our web site at neutrons.ornl.gov
- Contact the User Office. We will help you initiate your collaboration.
  - Judy Trimble, 865-241-3675 or trimblejl@ornl.gov

Sabbatical and Visitor Program

- Application should be prepared jointly with a proposed collaborator from ORNL
- Necessary for the applicant to supply a short statement describing the intended research
- Any visit to ORNL requires permission from the US Department of Energy.
- The typical maximum budgets are:
  (a) Faculty summer sabbaticals up to $40,000
  (b) Postdoctoral researchers up to $30,000 per year
  (c) Graduate students up to $20,000 dollars per year
- Instructions at http://neutrons.ornl.gov/crv/application.shtml

User Partnership Program for Sample Environment Equipment Development

- **New program to encourage the collaborative development of sample environment equipment; several productive collaborations already under way**
- **Interested users fill out a one-page template**
- **The scope is relatively small-scale (but high impact!) projects with a materials budget of $5K-$20K and some additional funds available to travel to ORNL**
- **Interaction between users and ORNL staff a key consideration, as well as a deliverable that will benefit the larger user program at SNS and HFIR**
- **More information at http://neutrons.ornl.gov/instruments/SNS/sample/**

EPSCoR travel grants

- **To carry out experiments at the Spallation Neutron Source and the High Flux Isotope Reactor at Oak Ridge National Laboratory**
- **For travels to discuss experiments before and after the measurements**
- **Available through The University of Tennessee for a limited number of faculty and students from EPSCoR institutions**
- **Contact Hope Moore-Webb, hmoore2@utk.edu, 865-974-1407 for details**
- **EPSCoR funding provided by the U.S. Department of Energy, Office of Basic Energy Sciences**

Of course there are regular jobs, to

Career Opportunities in Neutron Sciences at ORNL

Scientific Data Analysis Group Leader – Manages and leads the Scientific Data Analysis Group, a scientific software research and development group within Neutron Scattering Sciences Division that supports neutron scattering research conducted at the Spallation Neutron Source (SNS) and the High Flux Isotope Reactor (HFIR). Ensures an ongoing program of software development and maintenance that fully supports the data reduction and analysis needs of the SNS and HFIR beam lines.

Instrument Development Lead – Leads the continued modernization of operating instruments at SNS and HFIR, the development of new techniques on existing instruments, the development of new instruments at the existing facilities, and the development of instruments for new sources such as the SNS second target station and the HFIR second cold source. This leader must understand the scientific contributions possible through neutron scattering and have the vision to identify and lead new instrumentation initiatives to enhance scientific capability at SNS and HFIR.

Senior Scientists – Builds programs to drive the development of innovative scientific methods, tools, and technologies for neutron scattering research in targeted growth and development areas: energy materials (e.g., photovoltaics, catalysis, and solid-state materials), environmental geosciences (e.g., carbon sequestration and chemistry in extreme environments), nanostructured materials (e.g., soft matter, polymers, and self-assembly), and biological systems (bioenergy, biomembranes and structural biology). Senior Scientists are expected to develop partnerships that cut across the Neutron Sciences Directorate and other ORNL directorates, government agencies, universities, and industry.

Powder Diffraction Group Leader – Manages and leads the Powder Diffraction Group within Neutron Scattering Sciences Division and ensures the efficient operation and availability of the neutron scattering instruments. Organizes and leads efforts to continue development of instruments in the group to meet the changing scientific needs of the neutron scattering community.

Software Engineer – Develops highly advanced, multi-threaded software for data acquisition, in the form of Data Acquisition Systems GUIs for automating acquisition during neutron scattering experiments. Writes software for use with high-data-rate data acquisition and detector electronics.

Instrument Scientists – Helps users develop research proposals; conducts experiments and analyzes data; maintains the instrument and coordinates with support groups to ready it for each experiment; collaborates with staff and research groups at ORNL to conduct research using SNS and HFIR instruments; and conceives, plans, and executes instrument upgrades, including hardware and software.

Detector Scientist – Supports activities of the neutron scattering instruments in the user program, manufactures and installs detector systems for new instruments, and develops new neutron detectors for future applications. Provides high-level support for operating instruments, works with team members who build and install new systems, and successfully completes neutron detector research that benefits science in many fields, including research at neutron scattering facilities worldwide.

Sample Environment Team Lead – Establishes world-leading capabilities for temperature, pressure, and magnetic field environments for neutron scattering experiments and develops specifications and/or new designs, conduct hands-on assembly, testing, and debugging of the equipment, and train a technical team to become expert operators and troubleshooters.

To learn more about these opportunities, go to jobs.ornl.gov, or contact Tabitha Mase, masetc@ornl.gov, 865.576.0350

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ORNL is a multi program research facility managed by UT-Battelle for the U.S. Department of Energy. ORNL is an equal

Crystallograhy-Related Neutron Instruments at Oak Ridge National Laboratory

	Instrument (Beam Line)	Instrument Contacts	General Diffraction	Time-resolved[1]	Targeted Unit Cell Dimensions (Å)	Magnetic	Nanoparticles	Thin Films & Layers	PDF: Solids	PDF: Liquids/ Melts	Fiber	Texture Stress/strain	Diffuse/Off -specular Scattering	High Pressure	**Standard Sample Environments** D is displex temperature range, C is cryostat lowest temperature, Mh is horizontal magnetic field strength, Mv is vertical magnetic field strength, F is furnace temperature, SD is scheduled commissioning year, PR is pressure range, P is polarization
Neutron Powder Diffraction	NPD HFIR, HB-2A	Ovidiu Garlea, garleao@ornl.gov Clarina de la Cruz, delacruzcr@ornl.gov	•		<27	•			•					•	D(4 K-800K), C(1.5 K), Mh(0–6.5 T)
	WAND HFIR, HB-2C	Jaime Fernandez-Baca, fernandezbja@ornl.gov	•	•	<10	•			•					•	D(4 K-800K), C(1.5 K), Mh(0–5T), P(0.1-10 GPa)
	POWGEN SNS, BL-11A	Jason Hodges, hodgesj@ornl.gov Ashfia Huq, huqa@ornl.gov Olivier Gourdon, gourdonoa@ornl.gov	•	•	12	•						•			F(1200 K), PR, C, CF, D, Mv(16 T)
	SNAP SNS, BL-3	Chris Tulk, tulkc@ornl.gov Antonio Moreira dos Santos, dossantosam@ornl.gov		•	40	•								•	P (0-10 GPa; 26-900K)
	NOMAD SNS, BL-1A	Jörg Neuefeind, neuefeindjc@ornl.gov		•	12		•		•	•					SD=2010
	VULCAN SNS, BL-7	Xun-Li Wang, wangxl@ornl.gov Ke An, kean@ornl.gov Alexandru Stoica, stoicaad@ornl.gov	•	•	10	•	•		•	•	•	•			High precision (10 mm, 0.003 deg.) and heavy duty (up to 2 ton) sample positioning table. Multi-axial load frame with temperatures up to 1600 C.
	NRSF2 HFIR, HB-2B	Cam Hubbard, hubbardcr@ornl.gov	•		10							•			High precision d-spacing measurement and sample positioning system (to 1000 lbs) with laser
Single Crystal Diffraction	Four Circle HFIR, BL-3A	Bryan Chakoumakos, chakoumakobc@ornl.gov	•		<20	•			•				•		D(5-300K)
	TOPAZ SNS, BL-12	Christina Hoffmann, hoffmanncm@ornl.gov Xiaoping Wang, wangx@ornl.gov	•		<75	•		•					•		CF(4-600 K), P(3He incident beam polarization)
	MaNDi SNS, BL-11B	Leighton Coates, coatesl@ornl.gov	•		>50										SD=2013
	IMAGINE HFIR, BL4D	Flora Meilleur, meilleurf@ornl.gov	•		<100A	•			•					•	SD=2011
	CORELLI SNS, BL-9	Feng Ye, yef1@ornl.gov	•	•	<40								•		SD=2014
Small Angle Neutron Scattering	EQ-SANS SNS, BL-6	J. K. Zhao, zhaoj@ornl.gov		•	5-1500	•	•	•	•	•	•			•	CF: -5C to 200C
	General Purpose SANS HFIR, CG-2	Ken Littrell, littrellkc@ornl.gov Yuri Melnichenko, melnichenkoy@ornl.gov		•	5-1500	•	•	•	•	•	•			•	C: 1.5K-300K; CF: -5C to 200C; F: 30-1000C
	Bio-SANS HFIR, CG-3	Volker Urban, urbanvs@ornl.gov William Heller, hellerwt@ornl.gov		•	5-1500	•	•	•	•	•	•			•	CF:-5C to 200C
	U-SANS SNS, BL-1A	Michael Agamalian, magamalian@ornl.gov	•		1000Å-10μ	•	•	•	•	•	•			•	SD=2014
Reflectomters	Magnetism SNS, BL-4A	Valeria Lauter, lauterv@ornl.gov Haile Ambaye, ambayeh@ornl.gov			5										
	Liquids SNS, BL-4B	John Ankner, anknerjf@ornl.gov Jim Browning, browningjf@ornl.gov			5		•	•					•	•	PR to 1 kbar

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For additional information on ORNL instruments at the High Flux Isotope Reactor (HFIR) or the Spallation Neutron Source (SNS), please visit http://neutrons.ornl.gov.

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