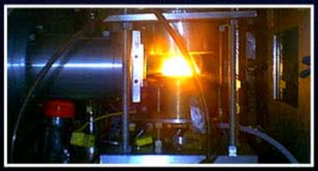
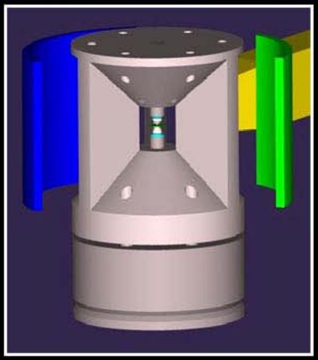
SENSE Workshop

Sample Environments for Neutron-Scattering Experiments

Workshop Report

Joint Institute for Neutron Sciences Workshop Series
Florida State University, Tallahassee, Florida
September 24-26, 2003





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SENSE

SAMPLE ENVIRONMENTS FOR NEUTRON SCATTERING EXPERIMENTS

Workshop Dates:
September 24-26, 2003

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Florida State University Center for Professional Development, Tallahassee, Florida

Sponsors:
National Science Foundation
University of Tennessee/Joint Institute for Neutron Sciences
Florida State University
Center for Nanophase Materials Sciences and Spallation Neutron Source/Oak Ridge National Laboratory
Oak Ridge Associated Universities

SENSE Workshop Organization:

Workshop Cochairs:

Prof. Jack Crow	National High Magnetic Field Laboratory/Florida State University
Prof. Paul Sokol	Pennsylvania State University

Program Committee (scientific and technical leadership):

Dr. Chris Benmore	Intense Pulsed Neutron Source/Argonne National Laboratory
Prof. Peter Liaw	University of Tennessee
Prof. Mathias Lösche	Johns Hopkins University
Prof. John Parise	SUNY Stony Brook
Dr. Thomas Proffen	Los Alamos Neutron Science Center/Los Alamos National Laboratory
Prof. Thomas Russell	University of Massachusetts
Prof. Ivan Schuller	University of California at San Diego
Prof. Barbara Wyslouzil	Worcester Polytechnic

Organizing Committee (logistics, administration, program committee assistance):

Mr. Lou Santodonato (Chair)	Spallation Neutron Source/Oak Ridge National Laboratory
Dr. Dan Dender	National Institute of Standards and Technology Center for Neutron Research
Dr. Al Ekkebus	Spallation Neutron Source/Oak Ridge National Laboratory
Dr. Linda Horton	Center for Nanophase Materials Sciences/Oak Ridge National Laboratory
Dr. Doug Lowndes	Center for Nanophase Materials Sciences/Oak Ridge National Laboratory
Prof. Lee Magid	University of Tennessee/Joint Institute for Neutron Sciences

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ACRONYMS

ANL	Argonne National Laboratory
CNMS	Center for Nanophase Materials Sciences
DOE	U.S. Department of Energy
FSU	Florida State University
HFIR	High Flux Isotope Reactor
HMI	Hahn-Meitner Institut
JINS	Joint Institute for Neutron Sciences
LANL	Los Alamos National Laboratory
LANCSE	Los Alamos Neutron Center for
NHMFL	National High Magnetic Field Laboratory
NIH	National Institutes of Health
NIST	National Institute for Standards and Technology
NRC	Nuclear Regulatory Commission
NSF	National Science Foundation
NSFChemBio	neutron scattering for chemistry and chemistry-biology interface
ORNL	Oak Ridge National Laboratory
R&D	research and development
SANS	small-angle neutron scattering
SE	sample environment
SENSE	sample environments for neutron-scattering experiments
SNS	Spallation Neutron Source

1. EXECUTIVE SUMMARY

1.1 WORKSHOP MOTIVATION AND OBJECTIVES

A growing number of scientists are using neutron-scattering techniques, and their research calls for an increasing range of sample environments (SEs) such as temperature, magnetic field, pressure, chemical environment, etc.. One objective of the Sample Environments for Neutron-Scattering Experiments (SENSE) Workshop was to gather input from the user community on major science drivers and to identify the associated SE needs. A further objective was to translate these needs into specific requirements and recommendations for future SE development. The ultimate goal was to provide guidance and encouragement for efforts to improve SE capabilities, ensuring a future of great science at neutron user facilities. This goal was addressed in collaboration with an overlapping workshop, Neutron Scattering for Chemistry and the Chemistry-Biology Interface (NSFChemBio). See www.sns.gov/jins/jins.htm for more information on the NSFChemBio workshop.

1.2 MAIN OUTCOMES

More than 150 scientists participated in the SENSE and NSFChemBio workshops, offering many valuable recommendations. Their strongest message was that SE equipment must be properly supported by people and site-wide infrastructure. Users expect direct assistance from a well-trained staff, including a dedicated SE team (rule of thumb: two SE team members per every $1M of equipment). User facilities also need to provide several types of sample preparation laboratories (deuteration facilities, mechanical areas, clean areas, wet chemistry tools, etc.). Another infrastructure issue, particularly for new facilities, is that neutron instruments must be designed with sufficient space for large SEs, abundant utilities, and nonmagnetic construction whenever possible.

Workshop participants also established many recommendations for developing a modern suite of SE equipment. It was recognized that each user facility takes sole responsibility for developing and supporting a "standard" equipment suite, but input from the user community is essential for shaping the makeup of that suite. Recommendations in this area include the need for modular designs that allow combinations of temperature, pressure, magnetic field, gas atmosphere, and pressure. To achieve high reliability, accuracy, fast response, and ease of use, the standard suite will likely cover moderate parameter ranges.

Many research areas require the development of specialized SE components, or complete systems, that extend the capabilities of the standard inventory. Wide varieties of in situ cells are needed to study biological and chemical processes, materials synthesis, and physical processes such as applied stress. Extreme temperature, pressure, magnetic field, and chemical environments are needed in areas such as catalysis, nano-magnetism, condensed matter physics, and planetary science. And new, high-flux sources will push the need to increase the speed and automation of SE systems. Workshop participants identified a range of these specialized needs and recognized the need for collaborations among users and facility staff to develop these concepts. Furthermore, there is a need to seek funding for specialized development projects that cannot be supported as part of the facility operating budget. However, it must be emphasized that specialized components and systems must ultimately be integrated with the standard inventories and that the ultimate responsibility for advancing neutron measurement capabilities, and SE capabilities, lies with the instrument scientists at the user facilities. These scientists must thus be encouraged to pursue both scientific and instrument development research and to form collaborations with experts throughout the user community.

1.3 OUTLINE OF MAJOR RECOMMENDATIONS

- The top SE priority for user facilities must be user support.
  - **People** dedicated to the direct support of users.
  - **Sample preparation laboratories**, including clean areas, wet chemistry tools, mechanical tools, deuteration facilities, etc., convenient to the beam line.
  - **Ample space and utility layout** at neutron instruments.

- Equipment priorities.
  - Standard suite (facility provided)—must have high reliability and accuracy, ease of use, and modular design allowing combinations of temperature, pressure, magnetic field, and gas environments.
  - Specialized/advanced equipment (facility/user-community collaboration).
    - Wide range of in situ environments including chemical, humidity, stress, and shear.
    - Extreme temperature, pressure, magnetic field, and chemical environments
    - Advanced automation and rapid response systems.

- The advancement of neutron measurement capability, and SE capability, ultimately rests on the instrument scientists at the facility.
  - Facilities must encourage staff research *and* equipment research and development (R&D).
  - Facility staff must seek collaborations with the user community and grants for specialized equipment development.

1.4 SENSE AGENDA OUTLINE

- Opening remarks
  - Purpose and goals of the workshop
  - Charge to participants

- Leading scientists from several communities speak about hot research topics with strong SE implications
- Poster sessions and tours of the National High Magnetic Field Laboratory (NHMFL)
- Instrumentation experts give a worldwide overview of SE capabilities
- Funding agency leaders discuss new and existing program initiatives
- User-facility panel
  - Facility leaders give brief status overview and future outlook
  - Discussion period

- Discussion panels establish priorities and recommendations for new SE development (5 parallel "breakout" sessions)
  - Quantum liquids and solids and other highly correlated electron systems
  - Polymers and macromolecules
  - Magnetism and nanosciences
  - Biological and life sciences
  - Materials evaluation and systematic studies of pressure, temperature, stress, etc.

- Breakout reports
  - Oral presentations given at the close of the workshop
  - Written reports included in this document

(The complete agenda is included in the appendix.)

2. INTRODUCTION TO THE BREAKOUT REPORTS

A key part of the information-gathering process took place during five parallel breakout sessions held on September 25, 2003. The session titles and chairs are listed subsequently.

2.1 BREAKOUT PANELS AND CHAIRS

Highly Correlated Electron Systems
Jeff Lynn, National Institute of Standards and Technology (NIST) Center for Neutron Research
Jack Crow, NHMFL/Florida State University (FSU)

Polymers and Macromolecules
Thomas Russell, University of Massachusetts
Greg Smith, Oak Ridge National Laboratory (ORNL)

Nanomagnetism and nanosciences
Frank Klose, Spallation Neutron Source (SNS)/ORNL
Mark Bird, NHMFL/FSU

Biological and Life Sciences
David Worcester, University of Missouri
Jim Torbet, University of Pennsylvania

Systematic Studies of Temperature, Pressure, Stress, . . .
Thomas Proffen, Los Alamos Neutron Science Center (LANSCE)
Takeshi Egami, University of Tennessee and ORNL

2.2 CHARGE

The sessions chairs and cochairs did an excellent job fulfilling their charge, which follows.

Goal: Establish SE requirements and recommendations based on the most important science drivers in your discipline.

How do we determine these drivers, requirements, and recommendations? These should begin to emerge from the plenary talks and discussions early in the workshop and continue to emerge during your session through a combination of targeted talks and discussions. As session chair, you should set the stage by stating the above goal, offering some preliminary views, introducing the short talks (more below), and wrapping things up with a discussion leading to a set of recommendations.

Practical Matters and Help:

Setting the stage: We will develop some standard opening slides for everyone to use.

Recruiting and inviting speakers: We will assist you in finding a few speakers (particularly for the chairs who recently came on board), sending invitations, and offering your speakers travel/lodging support (we can offer reimbursement for 2 to 4 speakers per breakout).

Session wrapup: You may wish to recruit plenary speakers and other experienced scientists to help lead the final discussion. In order to quickly draw useful information out of your group, ask some key questions, e.g., what's the most important scientific problem you would address using neutrons if only you had the right sample environment? (your input is encouraged regarding good wrap up ideas).

What are the guidelines for scheduling speakers and structuring the session? Much is left to your discretion, but begin your session at 3:30 p.m. with opening remarks, followed by talks, discussions, and wrapup. We have not put a time limit on the sessions, but schedule the time/number of speakers to allow a wrapup at a reasonable time (for example, 15-minute talks plus 5-minute question periods have been scheduled in one session).

The final step: Your findings will be reported during an open session on Friday morning, September 26, either by you or someone designated by you. The workshop organizers will distribute a final report in the weeks following the workshop.

2.3 REPORTS

The reports presented in the following chapters are based on the preliminary reports given by the session chairs on September 26, 2003.

3. BREAKOUT REPORT I: QUANTUM LIQUIDS AND SOLIDS AND OTHER HIGHLY CORRELATED ELECTRON SYSTEMS

Jeffrey Lynn, NIST Center for Neutron Research
Jack Crow, NHMFL/FSU

Forefront research on correlated electron systems often requires extremes in SE capability in order for the experimenter to tune the energetics of the system as data are collected. These types of experiments generally will push the SE frontiers, to be able to adjust thermodynamic variables over as wide a range as is practical. Experiments will require, for example, ultralow temperatures combined with high magnetic field capability, and/or high pressures. Other experiments will require investigation over a wide range of temperature, in addition to field and pressure. This area of research may be one of the more challenging areas for the SE capabilities of the facility. Following are aspects that we recommend be considered as the neutron instrumentation and SE facilities are developed.

3.1 OUTLINE OF NEEDS AND RECOMMENDATIONS (PRESENTED AT WORKSHOP CLOSEOUT)

- New, nonmagnetic instruments to accommodate large-field SE equipment. Asymmetric forces on the magnet caused by magnetic materials in the spectrometer particularly need to be avoided.
- State-of-the-art magnetic field capability, combined with state-of-the-art temperature and pressure capability.
- Easy-to-use, reliable field, temperature, and pressure SE systems. Many experiments do not necessarily need the ultimate in temperature range, field, etc., but rather the users need equipment that is flexible and robust, rather than state of the art.
- Magnetic field capability that uses incident and scattered polarized neutrons.
- Focusing beam optics that increase flux and thereby reduce the required sample size, particularly for magnetic field and pressure experiments. There is a tradeoff between maximum sample size design and ultimate capability.
- In situ measurement capability (e.g., magnetization, susceptibility, etc.) combined with the neutron measurements.
- Sample orientation capability in magnets and/or low/high temperatures.
- State-of-the-art high-pressure capability.
- Combined high-pressure, high-field, and wide-temperature range capability.
- Pulsed magnetic fields, either at SNS, or for time-dependent phenomena.
- Steady-state measurement capability and nonequilibrium capability.
- SE instrumentation capability that is matched with experienced personnel to maintain the equipment, prepare it for use, and assist scientists in its proper use.
- Support of instrument scientists to pursue their own research and extend measurement capability of the neutron instruments themselves and the SE. This is essential because advancement of neutron measurement capability, including SE capability, ultimately rests with the instrument scientists at the facility.
- Facility encouragement of funding opportunities for the development of new SE measurement capability involving collaborations between facility scientists and users.
- SE support at a level that allows inexperienced neutron users to come to the facilities and be successful in obtaining their measurements.
- Available software that allows users to quantitatively predict the cross sections to be measured and to predict how the SE will affect the measurement and the background.

4. BREAKOUT REPORT II: POLYMERS AND MACROMOLECULES

Thomas Russell, University of Massachusetts
Greg Smith, ORNL

This session brought together neutron scatterers interested in the studies of macromolecular systems, including polymers, liquid crystals, colloids, microemulsions, etc. The group identified several experimental sample parameters one would like to vary during neutron-scattering experiments on these materials. The environments were discussed in the context of small-angle neutron scattering, wide-angle diffraction, reflectometry, and spin-echo measurements. The types of SEs currently used in the studies of macromolecules were identified as well as environmental variables for future investigations. Once the pertinent, variable, and experimental parameters were identified, the corresponding SE equipment was categorized as "standard" (that which should be available at any neutron-scattering facility) and "desirable" (equipment that serves a limited group of users and that could exist at facility or that the user might have to supply). Finally, an integral part of the SE is the preparation labs. Discussions were held on the laboratory equipment required to support the SE efforts in the area of macromolecules.

We first examined the various types of environments and experiments of interest to scientists studying macromolecules. These included the following:

- **Temperature control:** This is a basic necessity for a variety of experiments from the basic control of the temperature of sample cells to control of cells with mK stability for measurements of critical phenomena.
- **Liquids:** Across the board, many of the fundamental measurements made on macromolecules are on liquid samples. These span the range from polymers in solution, to monolayers at liquid/air interfaces, to complex fluids in liquid or liquid crystalline phases.
- **High pressure:** Structure of and interactions between macromolecules can be measured as a function of applied pressure.
- **Supercritical fluids:** An emerging area of study is in the solvent properties of supercritical fluids on polymers. These experiments require a high-pressure apparatus to place the solvent (e.g., CO_2) in the supercritical phase.
- **Coupled fields:** Multiple fields can be applied simultaneously to a sample to study the combined effects of the environments.
- **Gradient fields:** Often one would like to measure structure as a function of an applied field where the field varies across the sample in a prescribed way. The sample is repositioned to measure various volumes of the sample.
- **In situ environments:** Environments were discussed that should be available for in situ studies, including the following:
  - Electrochemical
  - pH
  - Humidity
  - Processing
  - Electric, magnetic
  - Shear, flow

4.1 STANDARD EQUIPMENT

In the context of the previous discussion, the group turned to consider what equipment should be made available as a standard suite that a user can expect the facility to maintain and offer. The next level of information, namely the range of environmental parameters, was then discussed for each type of equipment to be provided. The list of standard equipment includes the following:

- Automatic sample changers: a series of samples in standard holders that can be measured where their temperature is maintained in a range of -60 to 400˚C.
- Dual temperature-controlled cells: The equilibration time can be longer than the experiment time. For measurements as a function of temperature, it would be desirable to have the samples equilibrated at several temperatures rather than waiting to change temperature on a single cell. This allows measurements of temperature jumps as well without long lead times.
- In situ ovens: vacuum or gas exchange to study the effects of exposure to a gas or to reduce oxidation.
- X,Y,Z-translation stages (independent of collimation): It is important to be able to select which region of the sample is to be studied and to accurately place the sample at that position.
- Liquid/solid cells (fluid exchange): For reflectometry experiments, these are basic to the studies of adsorbed monolayers in solution.
- Liquid/liquid cells (vibration isolation): The interface between two liquids can be studied with small-angle neutron scattering (SANS) or reflectometry.
- Cryostats/displexes: These standard pieces of equipment should be available for all instruments used to study soft matter.
- Magnets: Horizontal and vertical fields from 0 to 10 Tesla should be available for alignment of samples.
- Hydrostatic pressure cells: 0-6 kbar applied pressure either in the gas phase or liquid phase.
- Standard at-line utilities and services: water, gas, vacuum, and ventilation.

4.2 NOT-SO-STANDARD (BUT JUST AS IMPORTANT) EQUIPMENT

Another tier of equipment was identified that might not be available at all facilities but that should be available at least at a few select places. These items are generally requested by a smaller community of experimenters and/or could take a great deal of resources to operate and maintain. They include the following:

- Shear cells: couette geometry for SANS and Poiseuille flow geometry for reflectometers.
- Cone and plate shear cell/rheometers for reflectometers.
- Langmuir troughs for the study of materials at the liquid/air interface.
- A closed, humidity-controlled environment.
- Electric fields (DC, AC) both for macroscopic samples and thin films.
- Simultaneous capabilities in the scattering instruments themselves and nonscattering techniques simultaneously performed during the scattering experiments.
  - SANS and wide-angle neutron diffraction
  - Reflectivity and backscattering
  - Calorimetric measurements
  - Spectroscopic measurements
  - Rheological measurements

- Applied stress equipment
  - Solids (tensile, torsion, compression)

4.3 LABORATORIES

Finally, the last area for SE considered were the laboratories associated with the instruments and environments. It was recognized that in soft condensed matter experiments, the samples are often prepared on-site and loaded into the SE equipment on site or in situ. This makes it difficult to decouple support laboratory needs from the SE needs of the community. To this end, the group discussed those items that were deemed to be essential to support the SE needs for macromolecular research. These include the following:

- Clean areas free of dust and chemical contaminants.
- Hoods:
  - Solvent hoods for clean chemistry preparation.
  - Acid hoods for cleaning glassware.
  - Laminar flow hoods that provide a low level of airborne particulates. Some of these hoods should have spin coaters to prepare thin-film samples.

- A variety of small equipment, including:
  - Balances that are calibrated regularly to ensure accuracy.
  - Microscopes.
  - UV-ozone cleaners.
  - Vacuum ovens.
  - Standard wet chemistry tools.
  - Ultrapure water systems.

- Support: Laboratory technicians must be made available to help with the proper use of chemicals and equipment and with the proper disposal of chemical wastes.

5. BREAKOUT REPORT III: NANOMAGNETISM AND NANOSCIENCE

Frank Klose, SNS/ORNL
Mark Bird, NHMFL/FSU

The scope of the breakout session (attended by approximately 20 scientists, see subsequent list) was to provide neutron user facilities with a prioritized list of SE equipment that will be necessary for nanomagnetism and nanoscience experiments. To best address emerging opportunities, our group focused on the SNS magnetism reflectometer and the diverse community it will attract, particularly with the nearby Center for Nanophase Materials Sciences (CNMS). Certainly, other facilities and other types of neutron instruments will also play important roles in nanomagnetism and nanoscience research, and we hope that the following recommendations will be adapted and implemented by the larger community.

An important aspect of the following priorities is the distinction between "standard" and "specialized" equipment. As emphasized by SNS Experimental Facilities Division Director Ian Anderson at the opening of the SENSE Workshop, standard SE equipment will be provided (and funded) by SNS, but highly specialized equipment requires outside funding and collaboration between users and SNS staff. This type of collaboration is already under way, including efforts mentioned subsequently involving some of the SENSE participants. But we begin with a listing of standard equipment priorities, which are equally important to this field.

5.1 STANDARD SE EQUIPMENT FOR THE SNS MAGNETISM REFLECTOMETER

- Two- (or three-)dimensional field for reflectometry
  - a few Tesla along one direction
  - less along transverse directions
- Vertical split system for reflectometry and diffraction
  - up to 160° scattering angle for diffraction
  - NbTi (about 10 Tesla)
  - large bore (100 mm) for additional environmental control
  - complementary measurements
    - optical port for magneto-optical Kerr effect
    - resistivity/magnetoresistivity
- Helmholtz coil (10 to 100 Gauss)
  - for time-dependent and precision field measurements
- Temperature range
  - 1.5 to 1000 K (routine)
  - 10 mK (SNS shared cryostat)
- SE that fits inside magnet bore
- Optical port for LASER
- Controlled atmosphere inside sample chamber (high vacuum)
- Complementary sample characterization capabilities on-site at SNS and CNMS
  - Magnetometer, SQUID
  - X-ray reflectometer/diffractometer
  - etc.

5.2 SPECIALIZED SE EQUIPMENT

More specialized equipment is required for cutting-edge experiments making simultaneous use of the very high neutron flux at SNS and extreme sample conditions (very high magnetic fields, ultralow/ultrahigh temperatures, very high pressures, ultrahigh vacuum, etc.). It is expected that such specialized equipment facilitates revolutionary experiments that set new standards for science experiments at this next-generation spallation neutron source. Because such equipment will be used only by a small fraction of users, or maybe even solely dedicated to a particular user group, SNS expects that funding will be handled through separate proposals (U.S. Department of Energy, National Science Foundation, National Institutes of Health, etc.). A series of speakers presented their vision and scientific justification on state-of-the-art SEs.

5.2.1 LARGE BORE HIGH-FIELD MAGNET SYSTEM

Wai-Tung Lee (SNS/ORNL) and Mark Bird (NHFML, Tallahassee) presented requirements for magnetic fields. The highest priority item is a high-field magnet system:

- Vertical split systems 15-20 T
- Conical systems 20-25 T
- Transverse (horizontal) systems 10-15 T
- 2-D or 3-D systems 5-10 T

(Exact specifications to be determined by users based on availability of technology.)

The large bore will allow the setup to be used by a broad range of users by changing the insert with various special SEs and will ensure its flexibility to adapt for future developments in SE in the decades to come.

There was consensus that a configuration study should be carried out to optimize a high-field magnet system for neutron-scattering experiments. Electromagnetic, structural, and energy density limits for various configurations including detector/instrumentation should be addressed for making projections of performance, size, and cost to facilitate informed decision making.

5.2.2 UHV SYSTEM

Dongqi Li [Argonne National Laboratory (ANL)], Paul Miceli (University of Missouri, Columbia), and Rongyin Jin (ORNL) presented surface science research projects that require dedicated ultrahigh vacuum equipment. They emphasized that because of the extreme high neutron flux, surface science experiments with virtually monolayer resolution will become a real possibility at SNS. In contrast, current neutron-scattering instruments are able to resolve 10- to 20-Å films only. Preliminary specifications for the UHV system can be found in previous documents and white papers on the requirements for SE for the SNS magnetism reflectometer (these are listed subsequently and are available on request; e-mail Frank Klose at KloseFR@ornl.gov).

5.3 SESSION PARTICIPANTS

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5.4 SNS MAGNETISM REFLECTOMETER INSTRUMENT ADVISORY TEAM, REPORT ON SAMPLE ENVIRONMENT, JUNE 2000; PARTICIPANTS

Name	Organization
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John F. Ankner	SNS
Samuel D. Bader	ANL
Jack Bass	Michigan State University
Claude Fermon	CEA Saclay
Mike R. Fitzsimmons	LANL
John W. Freeland	Advanced Photon Source/ANL
Helmut Fritzsche	Hahn Meitner Institute, Berlin
J. Sam Jiang	ANL
Frank Klose	SNS
David Lederman	West Virginia University
Wai-Tung Lee	SNS
David Lind	FSU
Paul Miceli	University of Missouri
Andre Parizzi	SNS
Chris Platt	Seagate Research
James J. Rhyne	University of Missouri
Ivan K. Schuller	University of California, San Diego
Suzanne teVelthuis	ANL
Michael Toney	IBM Research Division

5.5 SAMPLE ENVIRONMENT SYSTEM PROPOSAL, *MAGNETIC NANOSTRUCTURES AND NEUTRON SCATTERING*, JAN. 2001; PARTICIPANTS

Name	Organization
Jack Bass	Michigan State University
Frank Klose	SNS/ORNL
D. M. Lind	FSU
Rainer Schad	University of Alabama

5.6 WHITE PAPER FOR *NANOMAGNETISM SAMPLE STATION FOR THE SNS POLARIZED NEUTRON REFLECTOMETER*, JULY 2002; PARTICIPANTS

Name	Organization
Mark Bird	NHMFL/FSU
Jack Crow	NHMFL/FSU
Axel Hoffmann	ANL
Frank Klose	SNS/ORNL
Chris Leighton	University of Minnesota
Rainer Schad	University of Alabama
Ivan K. Schuller	University of California, San Diego
Jian Shen	ORNL

5.7 PROPOSAL FOR *DEVELOPMENT OF HIGH-MAGNETIC FIELD SAMPLE ENVIRONMENTS FOR SNS AND HFIR*, SEPT. 2003 (DRAFT); PARTICIPANTS

Name	Organization
Mark Bird	NHMFL/FSU
Jack Crow	NHMFL/FSU
Frank Klose	SNS/ORNL
Andrey Zheludev	ORNL

6. BREAKOUT REPORT IV: BIOLOGICAL AND LIFE SCIENCES

David Worcester, University of Missouri
Jim Torbet, University of Pennsylvania

6.1 OUTLINE OF NEEDS AND RECOMMENDATIONS (PRESENTED AT WORKSHOP CLOSEOUT)

- Deuteration (essential)
- Relative humidity (accurately measured, well controlled, homogeneous)
- Sample changer with 10 to 20 positions, horizontal
- Hydrostatic pressure, ~5 kbar, Al or Ti/Zr and sapphire
- Magnetic Field for orientation, ~10T (cryogen free?)
- Hydrodynamic shear for orientations and rheology
- Pulsed electric fields for rotational diffusion
- Software control (as part of data acquisition)
- Ventilation for organics in reflectometry
- Langmuir trough

6.1.1 DEUTERATION OF BIOMOLECULES

Neutron-scattering studies in the biological sciences primarily use contrast variation and SANS together with specific deuteration of molecules or parts of molecules to determine arrangements and conformations of molecules in quaternary complexes. Such complexes are usually proteins but also include proteins in complex with nucleic acids or lipids. Selective deuteration of proteins is essential for many of these studies because it provides specific control of contrast to analyze arrangements and conformations of selected proteins within the complex. This makes the neutron-scattering experiments unique and gives scattering data that cannot be obtained with X rays or other techniques.

The essential need for deuterated biomolecules for neutron-scattering studies makes "in vivo" deuteration facilities a highest priority for biological studies with neutrons. Such in vivo deuteration was originally pioneered by Henry Crespi and Joseph Katz at ANL for nuclear magnetic resonance and infrared spectroscopy studies but later served the neutron-scattering community worldwide. Although larger research groups with sufficient resources developed their own deuteration facilities, smaller groups benefited greatly by the ready availability of deuterated material from ANL. Users of SNS for biological studies would similarly benefit greatly by the ready availability of deuteration resources. A substantial deuteration facility available to SNS users is therefore strongly encouraged. It should be readily accessible to SNS users to facilitate the development of projects.

6.1.2 CONTRAST VARIATION BY DYNAMIC NUCLEAR POLARIZATION

Although selective contrast variation in neutron scattering has traditionally been achieved by means of specific deuteration of macromolecules, coupled with measurements in different H_2O/D_2O solvent mixtures, there is another more advanced way that contrast variation can be achieved. This is the dynamic nuclear polarization technique first demonstrated by John Hayter and John White and later applied to biological macromolecules by Heinrich Stuhrmann (see H. B. Stuhrmann and K. H. Nierhaus in *Neutrons and Biology*, pp. 397-413, 1996). This technique makes use of the very different neutron-scattering amplitudes of hydrogen when the neutron and proton spins are parallel or antiparallel, respectively. It is therefore often called nuclear spin contrast variation. The dynamic nuclear polarization of samples makes this method technically very challenging; however, numerous results have been obtained. Sample conditions are T <1 K and magnetic fields of 2.5 Tesla, with specific microwave frequencies to provide dynamic polarization that is 70 to 90% for protons. For sample temperatures below 0.15 K, polarization persists for several weeks. This method should be applicable to determining proton configurations around active sites of enzymes.

6.1.3 RELATIVE HUMIDITY

For exploring phase space, relative humidity is a high priority among the membrane research community. The use of saturated salt solutions has been extensive but is not easily amenable to automated change of humidity, nor does it provide fine control of humidity for changes in small steps. Automated systems that provide these features have been developed, but improvements are desirable, especially for stability. Another key issue is accurate measure of relative humidity. Currently, this is only about ±3% and is often unsatisfactory. Convenient control of relative humidity, including to 100%, is needed. Good relative humidity control also requires temperature stability over the entire sample, so control and stability issues also apply to temperature, which in biology is generally in the range from about 0 to 70°C.

6.1.4 TEMPERATURE AND HYDROSTATIC PRESSURE

Special SEs commonly used in other sciences for exploring phase space are also useful in biology. These include hydrostatic pressure, which, like temperature, is a basic thermodynamic variable capable of affecting both phase behavior and macromolecular interactions. Pressure cells to 5 kbar are needed. These should be of two types: (1) aluminum or titanium/zirconium cells for membrane studies and (2) sapphire window cells for SANS studies of protein and other solutions. It is emphasized that protein interactions are a key aspect of biological processes, especially in the large and rapidly growing topic of signal transduction. Neutron scattering has been quite valuable in this area, where the key issues are not just structure but also the effects of changing conditions on protein complexes that are involved in cascades of events in living cells. Covalent changes such as phosphorylation and dephosphorylation are among the most significant changes that affect protein complexes, but temperature, pressure, and solvent conditions also are important.

6.1.5 ORIENTING BIOMATERIALS WITH MAGNETIC FIELDS

Many studies of biological molecules benefit from techniques that increase molecular orientation. Magnetic fields are especially useful for orienting fibrous structures, such as fibrin, actin, and microtubules, and for filamentous viruses and membranes. This magnetic field orientation is caused by the diamagnetic anisotropy of the peptide and ester bonds. Magnetic fields of at least 10 Tesla should be available for occasional use in biological work. The sample position usually needs to be room temperature or thereabouts. The possible use of cryogen-free magnets should be explored. It is emphasized that structure determination is not the only goal of studies using magnetic orientation. For membranes, changes of protein binding at the membrane surface are important aspects of signal transduction and issues of amplification associated with specific events can be addressed, as has been done with the rhodopsin and transducin system of visual processes.

6.1.6 HYDRODYNAMIC SHEAR WITH COUETTE GEOMETRY

Hydrodynamic shear with couette geometry has applications in biology, especially to membranes and lipids, as well as to cytoskeletal structures such as microfilaments, intermediate filaments, microtubules and fibrous complexes such as fibrin, the blood clot polymer. Effects of shear on such cellular structures are important in vivo, such as in the flow of blood cells through small capillaries whose diameters are less than those of the cells.

6.1.7 SOFTWARE CONTROL

Software control of sample conditions wherever possible is very important and should be part of the main data acquisition system. Sample changers are also essential and are widely used already because of the need for measurements in a variety of H_2O/D_2O mixtures, as well as other solvent conditions. Cooling of the sample changer is usually needed for sample preservation, and enclosure of the sample changer to avoid condensation problems is therefore imperative. Changers with 10 to 20 positions for quartz sample cells should be available for SANS.

For reflectometry studies in biology, ventilation at the sample position is needed for removal of organic solvent vapors. A Langmuir trough is also requested. An SE not specifically requested for biology, but that may find use at pulsed neutron sources is a pulsed electric field capability for orienting macromolecules in solution. Usually field strengths of about 1 kV/cm are used and must be pulsed to limit electrophoresis effects.

6.2 SESSION PARTICIPANTS

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7. BREAKOUT REPORT V: MATERIALS EVALUATION AND SYSTEMATIC STUDIES OF PRESSURE, TEMPERATURE, MAGNETIC FIELD, ETC.

Thomas Proffen, LANSCE/LANL
Takeshi Egami, University of Tennessee and ORNL

Cutting-edge research sometimes requires extreme environmental conditions, but it is often more important to have highly configurable environments that allow quick and accurate control of multiple parameters. The following recommendations reflect a demand for greater flexibility, accuracy, and efficiency. Sample changers, for example, are becoming increasingly important to allow users to fully exploit high-flux neutron instruments for systematic materials characterization. Background minimization and calibration of environmental parameters are other top priorities that often get too little attention but that are crucial for successful experiments. In situ studies are also of great interest, as demonstrated by some of the subsequent recommendations (e.g., chemistry reactor and control of sample atmosphere). Finally, some recommendations require the development of rather extreme capabilities, such as a load frame/furnace system that rivals today's best (SMARTS at LANL).

7.1 CHALLENGES AND SAMPLE ENVIRONMENT PRIORITIES

- Sample changers at low temperature and high temperature
- SE background as low as possible
- Load frame and furnace exceeding SMARTS capability (300 kN, 0.01 to 200 Hz)
- Control of sample atmosphere
- In situ chemistry reactor with possibility of probing (e.g., optical), temperature, and pressure
- Equipment calibration (T,P, etc.)
- Desired temperature range (by device type)
  - 1.5 K – RT (closed cycle refrigerators)
  - 4–900 K (cryofurnace)
  - RT–1500 K (furnace)
  - 1500–2400 K (HT furnace)
  - 0.03–4 K (dilution refrigerator)

- Accommodation of small samples and beam focusing to allow fast temperature change/equilibration.
- Sensors (attached to the sample holder)
- Sufficient feed-through connections to sample (user-configurable)
- Gas cells: 1 GPa, 1300 K
- Access to nonequilibrium liquids
- Loading capability 250 kN, 50 Hz
- Sample access from top and bottom
- Email survey of neutron users

7.2 SENSE WORKSHOP CONCLUSIONS

- The top SE priority for user facilities must be user support.
  - **People** dedicated to the direct support of users.
  - **Sample preparation laboratories**, including clean areas, wet chemistry tools, mechanical tools, deuteration facilities, etc., convenient to the beam line.
  - Ample space and utility layout at the neutron instruments.

- A wide range of equipment priorities were identified by the user community.
  - Standard suite (facility provided) must have high reliability and accuracy, ease of use, and modular design allowing combinations of temperature, pressure, magnetic field, and gas environments.
  - Specialized/advanced equipment (facility/user community collaboration).
    - Wide range of in situ environments, including chemical, humidity, stress, and shear.
    - Extreme temperature, pressure, magnetic field, and chemical environments.
    - Advanced automation and rapid response systems.

- The advancement of neutron measurement capability, and SE capability, ultimately rests on the instrument scientists at the facility.
  - Facilities must encourage staff research *and* equipment R&D.
  - Facility staff must seek collaborations with the user community and grants for specialized equipment development.

APPENDIX

COMPLETE AGENDA

NSFChemBio and SENSE Workshops
September 23-26, 2003
Turnbull Conference Center, Florida State University
Tallahassee, Florida

Sponsors

National Science Foundation
University of Tennessee/Joint Institute for Neutron Sciences
Florida State University
Oak Ridge National Laboratory/Spallation Neutron Source
Oak Ridge National Laboratory/Center for Nanophase Materials Sciences
Oak Ridge Associated Universities

Tuesday, September 23, 2003

7:00 am	Registration opens Vendor Exhibit Set-up
8:15	**Session N-I - Opening Session** Room 122
8:15	**Welcoming Remarks** Lee Magid, JINS Acting Director Jack Crow, NHMFL Director Art Ellis, NSF Chemistry Division Director
8:30	**Neutrons 101a: What Can Be Measured Using Neutrons,** John Root, NRC Canada
9:45	**Break, Fireside Lounge**
10:00	**Neutrons 101b: Instrumentation for Elastic and Inelastic Scattering Studies**, Kent Crawford, ORNL
11:00	**The European D-Lab Network**, Dean Myles, ORNL
11:30	**CNMS Facilities for Chemistry and Biology**, Mike Simonson, ORNL
12:00 pm	**A Neutron Scatterer's Dream: the Ideal Support Environment**, TBD
12:30	**Lunch, Room 121**

Tuesday, September 23, 2003 afternoon

1:30 pm	**Session N-2: Condensed Phases Room 123a** Chair: J. Martin	**Session N-3: Thin Films/Confinement Room 122,** Chair: J. Lal
1:30	**Water and Ice**, Alan Soper, ISIS	**Studying surfactant adsorption at interfaces by neutron reflectivity: the current 'state of the art' and future prospects**, Jeff Penfold, ISIS
2:00	**Unraveling Polymer Dynamics**, Michael Monkenbusch, Juelich	**Confined Complex Fluids**, Tonya Kuhl, University of California-Davis
2:30	**New Opportunities In Neutron Scattering: Local Sources and Novel Instrumentation**, David Baxter, Indiana	**Nanoporous Thin Films**, Shenda Baker, Harvey Mudd College
3:00	**Break, Fireside Lounge**	**Break, Fireside Lounge**
3:30	**Novel In-situ Studies**, TBD	**The Dynamics of Confined Quantum Tops**, Dan Neumann, NIST
4:00	**Dynamics of Materials**, Franz Trouw, Los Alamos	**Surface Adsorbed Films**, John Larese, University of Tennessee/Oak Ridge
4:30	**Discussion/Break**	**Discussion/Break**
5:00	**Session N-4, room 123a**	**Session N-5, Room 122**
5:00	**Advanced Isotopic Labeling Center and Facilities** (Dean Myles, Jeff Penfold)	**Educational Requirements and Opportunities** (Shenda Baker, Jim Martin, Joe Zwanziger)
6:30	**Session ends** **Buses Depart for Hotel**	**Session ends** **Buses Depart for Hotel**

Wednesday, September 24, 2003

7:00 am	Registration opens		
8:05	Vendor Exhibit Opens		**Session S-1 - Room 122 Science Drivers for Neutron Scattering: Impact of Enhanced Sample Environment** **Welcoming Remarks** Lee Magid, JINS Acting Director J. E. Crow, NHMFL Director
8:15			**Purpose and Goals of the SENSE Workshop**, Ian Anderson, Oak Ridge
8:30	**Session N-6, Room 123b Biological/Polymer Topics** Chair: J. Martin **3D Structure and Composites**, Ulrich Wiesner, Cornell	**Session N-7, Room 123a Catalysis/Vibrational Spectroscopy** Chair: J. Turner **Catalysis Studies Using TOSCA**, John Tomkinson, ISIS	**Nanomagnetism and Neutron Scattering**, Ivan Schuller, University of California – San Diego
9:00			**Quantum Liquids and Solids**, Paul Sokol, Penn State
9:15	**SANS Bio-polymer Studies**, Joanna Krueger, UNC-Charlotte	**The application of inelastic neutron scattering spectroscopy to advance the development of reaction mechanisms in heterogeneous catalysis**, David Lennon, Glasgow	
9:30			**Frontiers in High Pressure Science**, Russ Hemley, Carnegie Institution of Washington
10:00	**Break, Fireside Lounge**	**Break, Fireside Lounge**	**Break, Fireside Lounge**
10:30	**Organic-Inorganic Composites**, Josef Zwanziger, Dalhousie	**Novel Studies Using FANS**, Craig Brown, NIST	**Highly Correlated Electron Systems**, Zach Fisk, Florida State
11:00	**Polymer Patterned Surfaces**, Jan Genzer, NCSU	**Novel Studies Using FDS**, Luc Daemen, Los Alamos	**Materials Science and Engineering Studies Using Neutron Diffraction**, D. W. Brown, Los Alamos

11:30	**Neutron Spectroscopy and Molecular Dynamics Simulation Studies of Protein Dynamics**, Doug Tobias, UC-Irvine	**Nanocomposites for electronic and biomedical applications,** Chris Durning, Columbia	**Three-Dimensional Neutron Microscopy for Structural Dynamics Investigations**, Ben Larson, Oak Ridge

Wednesday, September 24, 2003

Wednesday, September 24, 2003 Afternoon

	Combined Session of NSFChemBio and SENSE
1:00 pm	**Sessions N-8 and S-2, Room 122** **Beyond Traditional Neutron Science** **Biological and Chemical Science Opportunities at the Center for Nanophase Materials Science**, Mike Simonson, Oak Ridge
1:30	**Dynamic Structure of Membranes: The Concerted Use of Bi-layer Diffraction and Molecular Dynamics Simulations**, Stephen H. White, University of California – Irvine
2:00	**Synchrotron X-ray Studies of Liquid Surfaces**, Peter Pershan, Harvard
2:30	**Extreme Environments for Catalysis**, John Turner, University of Tennessee
3:00	**Break, Fireside Lounge**
3:30	**Environments for Biological Studies**, John Katsaras, Chalk River
4:00	**Polymers and Macromolecules**, Tom Russell, University of Massachusetts
4:30	**Investigation of Liquid Surfaces**, Jarek Majewski, Los Alamos
5:00	**Chemical Reaction Dynamics of Aerosols**, Barbara Wyslouzil, Worcester Polytechnic Institute
5:45	**Depart for National High Magnetic Field Laboratory** **Poster Session and Tour** **Buses Provided from Turnbull to the NHMFL and return to Turnbull and the hotels**
8:30	**Poster session and tour over** **Buses return to Turnbull and Hotels**

Thursday, September 25, 2003

7:00 am	**Registration open**		
8:30	**Session N-9, Room 123a Future Opportunities and Needs: Support Facilities Needs for Soft Matter** (Paul Butler, Joanna Krueger)	**Session N-10, Room 123b Future Opportunities and Needs: Support Facilities Needs For Hard Matter** (John Larese, John Turner)	**Session S-3, Room 122 Present Status of Neutron Sample Environments at High Magnetic Fields and Low Temperatures**, Michael Meissner, HMI, Berlin
9:00			**Research Capabilities at High Pressure**, Chris Tulk, Oak Ridge
9:30			**High Temperature Capabilities**, Trudy Kriven, University of Illinois, Urbana-Champaign
10:00	**Break, Fireside Lounge**	**Break, Fireside Lounge**	**Break, Fireside Lounge**

10:30 am	**Sessions N-11 and S-4, Room 122** **Funding Opportunities and New Program Initiatives**
10:30	**New Funding Programs for Mid-Scale Projects and International Cooperation**, Tom Weber, National Science Foundation
11:00	**What's New in DOE's Neutron Scattering Program** Helen Kerch, DOE
11:30	**Funding Opportunities at National Institutes of Health**, Michael Marron, NIH
Noon	**Lunch** **Registration closes**

1:00 pm	**Sessions N-12 and S-5, Room 122** **Current Opportunities for Interfaces to Neutron Scattering Research and Education** **National Science Foundation International Materials Institutes (IMI) Program, Advanced Neutron Scattering netWork for Education and Research: with a Focus on Mechanical Behavior of Materials**, P. K. Liaw, University of Tennessee
1:30	**Sessions N-13 and S-6, Room 122** **Current Neutron Scattering and Sample Environment Capabilities**
1:30	**Enabling 21st Century Science**, Zoe Bowden, ISIS
2:00	**Panel Discussion: Thoughts on Current Sample Environment Capabilities and Future Needs at North American Facilities** **Chalk River,** Canada, John Katsaras **High Flux Isotope Reactor**, Oak Ridge, Greg Smith **Intense Pulsed Neutron Source**, Argonne, Ray Teller **Los Alamos Neutron Scattering Center**, Los Alamos, Alan Hurd **NIST Center for Neutron Research**, NIST, Jeff Lynn **Spallation Neutron Source**, Oak Ridge, Thom Mason
3:00	**Break, Fireside Lounge**

Thursday, September 25, 2003

Parallel Sessions: Establishing Sample Environment Priorities

Short presentations will be followed by group discussions; summaries of these discussions will be presented Friday morning in session S-8.

3:30 pm	**Panel I, Room 123a: Sample Environment Priorities in Nano-Magnetism and Nano-sciences.** Chair: Frank Klose, Oak Ridge	**Panel 2, Room 115: Sample Environment Priorities in Biological and Life Sciences.** Chair: David L. Worcester, University of Missouri - Columbia	**Panel 3, Room 123b: SE Priorities for Quantum Liquids and Solids and Other Highly Correlated Electron Systems.** Chair, Jeff Lynn, NIST	**Panel 4, Room 110: Sample Environment Priorities for Polymers and Macro-molecules**. Chair, Thomas Russell, University of Massachusetts	**Panel 5, Room 122: Sample Environment Priorities for Materials Evaluation and Systematic Studies of Pressure, Temperature, Stress, Etc.** Chair, Thomas Proffen, Los Alamos
	In-situ X-ray Scattering Studies of Epitaxial Crystal Growth, Paul F. Miceli, University of Missouri – Columbia	John Katsaras, Chalk River	Alex Lacerda, NHMFL, Los Alamos	Greg Smith, HFIR, Oak Ridge	**Assembling and Studying Metastable Materials Using Containerless Techniques**, Richard Weber, Containerless Research
	Self-assembly of Epitaxial Magnetic Nanostructures, Donqi Li, Argonne	Stephen H. White, UC-Irvine	Michel Kenzelmann, NIST and Johns Hopkins	Lee Magid, University of Tennessee/ JINS	**Conventional Sample Environment Challenges**, Takeshi Egami, University of Tennessee/ORNL
	Studies of Magnetic Nanostructures Using Polarized Neutrons – Current Status and Future In-situ Studies, Hal Lee, ORNL	Jim Torbit, University of Pennsylvania	Meigan Aronson, University of Michigan		Chris Benmore, Argonne
	Opportunities for Magnetic Field Sample Environments for Neutron Scattering, Mark Bird, National High Magnetic Field Lab				
	Pushing Science Frontiers with state-of-the-Art Sample Environment, Rongying Jin, Oak Ridge				
5:30 pm	**Session ends** **Bus departs for Hotel**				

Friday, September 26, 2003 Morning

7:00 am	**Turnbull Conference Center Opens**
8:30	**Session S-8, Room 122** **Establishing Sample Environment Priorities: Discussion of Recommendations from Breakout Sessions**, Chair, Jack Crow, Florida State University
8:30	**Panel 1 Report: Sample Environment Priorities in Nano-Magnetism and Nano-Sciences**, Frank Klose, ORNL
9:00	**Panel 2 Report: Sample Environment Priorities in Biological and Life Sciences**, D. Worcester, University of Missouri
9:30	**Panel 3 Report: Sample Environment Priorities for Quantum Liquids and Solids and other Highly Correlated Electron Systems**, Jeff Lynn, NIST
10:00	**Break, Fireside Lounge**
10:30	**Panel 4 Report: Sample Environment Priorities for Polymers and Macro-molecules**, Thomas Russell, University of Massachusetts
11:00	**Panel 5 Report: Sample Environment Priorities for Materials Evaluation and Systematic Studies**, T. Egami, University of Tennessee
11:30	**Summary of Panel Recommendations**
12:00	**Adjourn and Box Lunch Provided**

12:00	**Begin with Working Lunch** **Session S-9, Room 122** **Technical Workshop, Follow-up to the April 2001 Workshop at PSI** Chair, Ken Volin, Argonne
12:00	**Sample Encapsulation Considerations in Designing High Temperature Neutron Diffraction Experiments**, Ken Volin, Argonne
12:20	**Trials and Benefits of Implementing a Computerized Maintenance Management System for Sample Environment Groups,** Joe Fieramosca, Argonne
12:40	**Do we still need helium-flow cryostats?** Frederic Thomas, Institut Laue Langevin
1:10	**Twin solution dilution refrigerators**, Ton Konter, Paul Scherrer Institute, Switzerland