Second Target Station Workshop Report

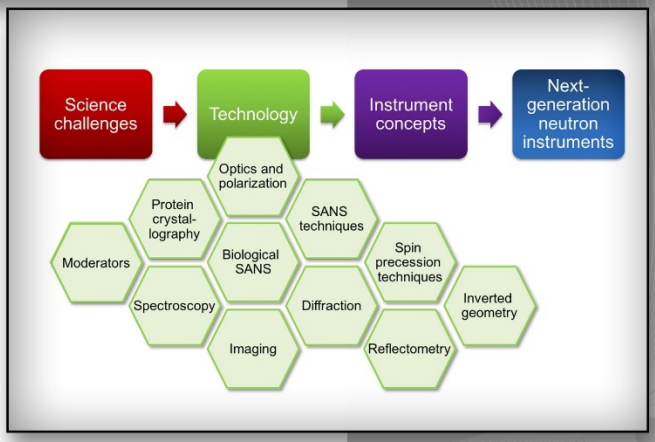

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Table of Contents

ABBREVIATIONS, ACRONYMS, AND INITIALISMS

3D	3-dimensional
AC	alternating current
DNP	dynamic nuclear polarization
DOE	Department of Energy
DYPol	dynamically polarized crystallography
ESS	European Spallation Source
FI	ferromagnetic insulator
FTS	first target station
FWHM	full width at half maximum
GID	grazing incidence diffraction
GI-SANS	grazing incidence small angle scattering
GINS	grazing incidence neutron scattering
HFIR	High Flux Isotope Reactor
Hz	Hertz
IDPs	intrinsically disordered proteins
IDRs	intrinsically disordered protein regions
ILL	Institut Laue-Langevin
INS	inelastic neutron scattering
IR	infared
J-PARC	Japan Proton Accelerator Research Complex
LDRD	Laboratory Directed Research and Development
MPB	morphotropic phase boundaries
MOKE	Magneto Optic Kerr Effect
NHMFL	National High Magnetic Field Laboratory
NMR	nuclear magnetic resonance
NIST	National Institute of Standards and Technology
NR	neutron reflectometry
NScD	Neutron Sciences Directorate
NSE	neutron spin echo
NVS	neutron vibrational spectroscopy
ORNL	Oak Ridge National Laboratory
PDF	pair distribution functions
PI	principal investigator
QENS	quasielastic neutron scattering

RIXS	resonant inelastic x-ray scattering
RTILs	room-temperature ionic liquids
SANS	small-angle neutron scattering
SDPD	structure determination from powder diffraction
SEI	solid-electrolyte interphase
SHUG	SNS HFIR User Group
SLD	scattering length density
SM	standard model
SNS	Spallation Neutron Source
SPLEED	spin-polarized low energy electron diffraction
STS	Second Target Station
T	Tesla
TDR	Technical Design Report
TIs	topological insulators
TIE	Transport-of-Intensity equation
TOF	time of flight
UCN	ultracold neutrons
UV	ultraviolet
UV-vis	ultraviolet visible
VCN	very cold neutron
WLSF	wavelength shifting fiber

Instrument Names

ARCS	Wide Angular-Range Chopper Spectrometer
BASIS	Backscattering Spectrometer
BIO-SANS	Biological Small-Angle Neutron Scattering Instrument
CNCS	Cold Neutron Chopper Spectrometer
CORELLI	Elastic Diffuse Scattering Spectrometer
EQ-SANS	Extended Q-Range Small-Angle Neutron Scattering Diffractometer
FNPB	Fundamental Nuclear Physics Beamline
HYSPEC	Hybrid Polarized Beam Spectrometer
IMAGINE	Image-Plate Single-Crystal Diffractometer
IMAGING	Neutron Imaging Prototype Facility
Liq Ref	Liquids Reflectometer
MaNDi	Macromolecular Neutron Diffractometer
Mag Ref	Magnetism Reflectometer
NOMAD	Nanoscale-Ordered Materials Diffractometer
NRSF2	Neutron Residual Stress Mapping Facility
NSE	Neutron Spin Echo Spectrometer
POWGEN	Powder Diffractometer (SNS)
SEQUOIA	Fine-Resolution Fermi Chopper Spectrometer
SNAP	Spallation Neutrons and Pressure Diffractometer
TOPAZ	Single-Crystal Diffractometer
VISION	Vibrational Spectrometer
VULCAN	Engineering Materials Diffractometer

Proposed Instruments

BWAVES	Broad-range Wide Angle Velocity Selector
CAMEA	Indirect time of flight spectrometer
CHESS	Chopper Spectrometer for Small Samples
EWALD	Enhanced Wide Angle Laue Diffractometer
FLOODS	Flux-Optimized Order/Disorder SANS
HERTZ	High Energy Resolution Terahertz Spectrometer
HighResPD	High-Resolution Powder Diffractometer
HiResSWANS	High Resolution Small/Wide Angle Neutron Scattering
JANUS	Inelastic scattering instrument (INS) Instrument for Catalysis
MANTA	Multiple Analyzer Triple-Axis
MBARS	Mica Backscattering Spectrometer
MENUS	Materials Engineering by NeUtron Scattering
M-STAR	Magnetism-Second Target Advanced Reflectometer
nEDM@STS	neutron electric dipole moment (EDM) experiment at the second target station
NeSCry	Neutron Single Crystal Diffractometer
POPCORN	Polychromatic Phase-Contrast Neutron Imaging
QIKR	Quite Intense Kinetics Reflectometer
RAPID	Rapid Acquisition Parametric and In-situ Diffractometer
SPHIINXS	Spherical Indirect Inelastic Crystal Spectrometer
VBPR	Variable Beam Profile Reflectometer
VENUS	Versatile Neutron Imaging Instrument at the SNS
VERDI	Versatile Diffractometer for Complex Magnetic Structures
WASABI	Wide And Small Angles with Big Intensity
XTREME-X	Extreme Environment Multi-Energy Spectrometer with Crystal Analyzers
ZEEMANS	High Magnetic Field Beam Line

1. WORKSHOP SUMMARY

Neutron scattering is an essential tool for scientists studying the relationships between structure, dynamics and function of materials, from batteries and superconductors to polymers, enzymes and complex cellular machines. The understanding obtained by this technique allows researchers to form predictive models that inform the design of new and complex materials, which is essential to maintain U.S. competitiveness in the global marketplace. To fully realize the potential of this field of research and support the growing neutron scattering community, it is critical to maintain and expand the national neutron science facilities.

Oak Ridge National Laboratory (ORNL) is a leading center for neutron sciences worldwide, with the mission to ensure that the nation is served with cutting-edge capabilities for undertaking research that addresses the needs of the Department of Energy (DOE), as well as the broader community. As part of this mission, the Neutron Sciences Directorate (NScD) has undertaken, in consultation with the sponsors and science community, an in-depth look at the major needs for neutron sciences and areas of significant impact spanning the next decade and beyond. A central part of this process has been the formation of four high level science-themed, Grand Challenges workshops to delineate emerging and future challenges, and identify priority areas where developments in neutron sciences are most needed. This effort has been complemented by the formation of a series of working groups charged with exploring how these challenges could be addressed. A key conclusion of these discussions is that the proposed second target station (STS) is necessary at the ORNL Spallation Neutron Source (SNS), and that it will create new opportunities as the first Fourth Generation Neutron Source, while complementing existing sources at ORNL. The work carried out by NScD is summarized in a report entitled "Instrument for Emerging Science: A Science Case for the Second Target Station" and the accompanying Technical Design Report (TDR).[1]

The Second Target Station Workshop was organized by the Executive Committee of the SNS HFIR User Group (SHUG), and held at ORNL, October 27–29, 2015. The purpose of the workshop was to update the user community on the background and planning for the STS, to seek the community's input on all aspects of the project, and to engage the users in the process of moving the STS forward. The workshop was well attended, with 196 registered participants distributed as follows: 91 external, 87 from NScD, and 18 from other ORNL divisions.

The first half-day was used to update the user community on the background for and status of the STS project, and how the STS will complement the existing neutron sources at ORNL. This included presentations on the planned STS characteristics and summary talks outlining the main outcomes of the four Grand Challenges workshops that provided the scientific motivation for the STS project. Gains in performance of two orders of magnitude and beyond over existing capabilities makes the STS transformative for many of the research areas identified during these workshops. These gains result from a combination of technological developments, including advances in target and moderator technology, as well as recent developments in neutron optics where lensing, guiding, and wavelength analysis are all taking major steps forward. In addition, advances in manipulation of the spin of electrons, nuclei, and neutrons allow *in situ* control of scattering cross sections and contrast, and revolutionize what can be measured in magnetic and hydrogenous materials. Finally, high performance computing will enable reconstruction and analysis of multimodal data and simulation of systems gluing together disparate data sets and open complex scenarios to analysis and interpretation. Taken together, these define STS as a new generation of neutron facility of far reaching science impact.

[1] Instruments for Emerging Science: A Science Case for the Second Target Station, ed. K. W. Herwig and D. A. Tennant, Neutron Sciences Directorate, ORNL 2014 (unpublished); Technical Design Report Second Target Station, ORNL/TM-2015/24, January 2015.

The main component of the STS workshop was a full day of breakout sessions focused on the following two areas:

- Discussion and further development of the scientific case for the STS.
- Identification of the necessary performance parameters for the initial suite of instruments and how to achieve these "must reach" specifications.

The breakout sessions were organized according to scientific areas in the morning and according to instrument classes in the afternoon (see Appendix 1 for workshop agenda). Prior to the workshop, participants received separate science and instrumentation worksheets to prepare for the discussions (see Appendix 2). An important component of the STS project is the ability to reach out into new science areas and bring whole areas of science, such as biology and materials chemistry, into reach where the unique properties of neutrons can then play as important a role as they do today for quantum condensed matter and soft materials.

The final half-day began with summaries by discussion leaders, presenting results of the breakout sessions for all the workshop participants. In all cases, session chairs reported engaged and vigorous discussions. In particular, there was a unanimous strong support for the three-source strategy, outlining the need for the three complementary neutron sources at ORNL, the High Flux Isotope Reactor (HFIR) and the first and second target stations at the SNS. There was also a sense that the overall design of the STS should be science driven, focusing on the high level scientific and societal objectives rather than specific beam line or technique considerations.

The workshop concluded with an open town hall discussion to prioritize the proposed instrument concepts, and select the ones that will be further developed as candidates for the initial suite of instruments at STS. These instruments are:

- Indirect geometry spectrometer with high energy resolution and a very broad dynamic range of energy transfers (BWAVES)
- Cold neutron chopper spectrometer optimized for very small samples (CHESS)
- Enhanced wide angle Laue diffractometer optimized for small macromolecular single crystals and with dynamic neutron polarization (EWALD)
- High resolution powder diffractometer (HighResPD)
- Hybrid indirect/direct geometry spectrometer optimized for irreversible phenomena and *in situ* sample manipulation (JANUS)
- Kinetics reflectometer optimized for rapid specular reflectivity measurements from a horizontal sample (QIKR)
- Indirect geometry spectrometer optimized for ultra-high energy resolution studies (MBARS)
- Materials engineering by neutron scattering (MENUS)
- Reflectometer optimized to deliver a variable beam profile onto a sample surface as small as 1 mm^2 and for magnetic studies (M-STAR/VBPR)
- Combined small-angle neutron scattering (SANS)/diffractometer optimized for structural studies from molecular to tens of nanometers (HiResSWANS)

- Diffractometer optimized for magnetic structure studies of both powder and single crystals (VERDI)
- Versatile instrument that integrates neutron spectroscopy, diffraction, reflectometry and SANS with a very high field magnet (ZEEMANS)

Members of the user community interested in the further development will be invited to join instrument advisory teams.

In conclusion, the STS will ensure the United States leads in neutron sciences for the foreseeable future. The availability of the above instruments, as well as others to follow, will dramatically enhance the understanding of materials from the atomic to real world scales. It will provide unprecedented access to mesoscale quantum and complex matter, and ensure that the unique contributions of neutrons to discovery and understanding in these fields continue for decades ahead.

2. INTRODUCTION AND BACKGROUND

ORNL is a leading center for neutron sciences worldwide with the mission to ensure that the nation is served with cutting-edge capabilities for undertaking research that addresses the needs of DOE, as well as the broader community. Significant investments by DOE have provided the nation with two forefront neutron scattering facilities located at ORNL, the SNS and HFIR. The ORNL NScD currently offers general user community access to 30 neutron scattering instruments across these two facilities that supported 1252 experiments in Fiscal Year (FY) 2015. NScD has undertaken, in consultation with the sponsors and science community, an in-depth look at the major needs for neutron sciences and areas of significant impact spanning the next decade and beyond. A central part of this process was the formation of four high-level science-themed Grand Challenges workshops held late 2013 through 2014 to delineate emerging and future challenges and to identify priority areas where developments in neutron sciences are most needed. This effort was complemented by the formation of a series of working groups charged with exploring how these challenges could be addressed. A key component is the proposed STS at the SNS, which will create new opportunities for neutron sciences.[1]

2.1 FUTURE SCIENCE NEEDS FOR NEUTRONS AND THEIR ROLE

To identify emerging science where neutrons are an essential tool as well as the needs of the community, the four workshops addressed the future of quantum condensed matter, soft matter, biology, and the frontiers in materials discovery. These workshops provided a host of compelling scientific and technological challenges for the decade ahead that are inaccessible to other techniques or where the contribution of neutrons in combination with other techniques is vital. They also identified areas where a step change in capabilities is needed. In nearly all cases, the primary capability gaps that need to be addressed require more intense beams in the long wavelength (“cold”) regime and for instrumentation using a large bandwidth. The 10 hertz (Hz) STS source described in the TDR[1] and described in Appendix 3 will provide unparalleled neutron peak brightness and dynamic range for long wavelength cold neutron applications. Indeed, the capabilities envisaged will make this a truly next generation facility, and together with the first target station (FTS) and HFIR reactor source, the STS facility will ensure U.S. capabilities that go beyond any existing or planned sources worldwide for the next generation.

2.1.1 Quantum Materials[2]

Although normally associated with physics at the atomic scale, quantum coherence can give rise to spectacular properties when it transcends the atomic scale through collective behavior in so called quantum materials. Neutrons provide access to the spatial and temporal electronic correlations and have played a pivotal role in our rapidly developing understanding of these materials.

The workshop on Quantum Condensed Matter examined the current state of research on quantum materials, how the field might evolve over the next decade, and the role of neutron scattering in these developments. It also covered the synthesis of new materials, the complementary use of neutrons and x-rays, and included discussion of the roles of muons and high magnetic fields. Overall, the scientific field of quantum condensed matter is found to be uncovering a rich variety of collective phenomena, some of which present exciting opportunities for technological impacts, and neutron scattering was determined to be an absolutely central technique for progress in the field.

The workshop highlighted a number of crucial problems in quantum materials research where neutrons are indispensable. These problems range from understanding the exotic ground states that emerge in quantum spin systems, quantum critical phenomena, topological states of matter, and quantum materials out of equilibrium, to the physics underlying unconventional superconductors and itinerant magnets.

Increasingly, quantum materials are poised to make a major technological impact both in information technologies and energy. Progress in new devices and spintronics in particular require advances in neutron capabilities for probing structure and dynamics in thin films/heterostructures/nanomaterials. The importance of the special properties of strongly correlated states in energy storage and conversion are now being recognized and open up new needs for diffraction and inelastic neutron scattering (INS).

A major trend in the coming years is the increasing importance of mesoscale phenomena for controlling properties. These techniques will require spatially-resolved probes of (especially magnetic) structure of materials on the sub-micron scale, as well as determination of the structure of partially ordered materials including defect structures.

2.1.2 Soft Matter[3]

One of the goals of modern science is to create materials by design with specific functionalities. Soft matter composed of covalently bound molecular building blocks (including polymers, surfactants, nanoparticles, gels, etc.) provides almost endless complexity and tunability for making new materials to achieve this goal. As the complexity of these systems grows, so do the challenges for developing the fundamental understanding of the materials' properties with the ultimate goal of controlling static and dynamic function.

Areas of compelling scientific need where neutrons will play a key role have been established. These extend into the response of soft matter to mechanical deformation, soft/hard composite materials, interfaces, and transport in soft matter. Also of fundamental need are capabilities to understand polar solvents other than water, polyelectrolytes, and complex structures in solution such as hierarchical assemblies. The widespread impact of soft matter technologies will require looking at soft matter under

[2] Based on the report of the Quantum Condensed Matter Workshop, December 5–6, 2013, Lawrence Berkeley National Laboratory, R. J. Birgeneau (University of California, Berkeley).
[3] Report from "Grand Challenges in Soft Matter" Workshop May 17–18, 2014, University of California, Santa Barbara, P. A. Pincus (University of California, Santa Barbara) and M. Tirrell (University of Chicago).

industrial processing conditions, understanding active soft materials, expanding the ability to make quantitative measurements, and gaining insight into the effects of poly-dispersity on physical properties.

While neutrons are an essential tool for studying soft matter today, in the future, new techniques and new sources will provide even more information on these complex systems. The proposed STS will be optimized to provide a high flux of long wavelength neutrons over a wide bandwidth. It will be ideally suited to simultaneously studying multiple temporal and spatial scales, which are crucial to understanding complexity in soft systems. To exploit and fully interpret the data, a closer coupling between modeling and experiment will be essential. Significantly increased facilities for selective isotopic labeling (primarily deuteration) will be needed. Soft matter has a growing synergistic relationship with molecular and cellular biology in the area of synthetically reproducing and enhancing the functionality found in living systems. Achieving these goals may involve the marriage of synthetic and biological moieties.

2.1.3 Biology[4]

Gaining a predictive understanding of the behavior of complex biological systems is one of the greatest scientific challenges that will be faced over the next decade. This understanding will guide in protecting and repairing physiological systems; it will allow the mimicking of the architectures and processes of living systems to create new biomaterials and bio-inspired technologies; and it will provide the information necessary to manipulate micro-organisms and their ecosystems to create new biotechnology and biorefinery solutions to emerging energy and environmental challenges.

Neutrons provide several types of unique information that will be important in addressing future problems and are poised to have major potential impacts, including influence on membrane associated biological processes and the dynamic assembly and regulation of large biological complexes. Neutrons provide direct access to crucial processes through their high sensitivity to hydrogen, which drives the chemistry and physics of living systems, in conjunction with isotopic substitution with deuterium, which enhances the visibility of specific parts of complex biological systems. The application of neutrons is being opened up by high performance computing simulations, which allow for prediction and interpretation of data from systems that are too complex for analytical theory. Neutrons are also complementary to techniques using photons and electrons. Photons and electrons interact with the atomic electric field and are most sensitive to heavy atoms; but with just one electron, hydrogen is all but invisible. Neutrons interact with nuclei so light atoms such as hydrogen are highly visible. In addition, neutrons cause little radiation damage and are highly penetrating, enabling the use of complex sample environments.

Despite the advantages in using neutron scattering, significant technical gaps must be bridged not only in neutron scattering instrumentation but also in sample preparation using molecular biology and deuterium labeling, and in post-acquisition analysis using computational technologies. They include the need for more advanced deuterium labeling techniques, better access to neutron beam lines, increased neutron flux, beam lines optimized for membrane diffraction, the development of innovative techniques for polarizing neutron beams and hydrogen atoms in samples to enhance scattering power and to dynamically control scattering contrast, and the development of new instrumentation that allows simultaneous access to broad regions of time and space. In addition, better integration of high performance computing techniques with neutron scattering experiments, and the development of computational tools that allow the combination of experimental data from multiple complementary techniques to generate more complete models of complex biological systems are needed.

[4] Report from "Grand Challenges in Biological Neutron Scattering" Workshop January 17–18, 2014, University of California, San Diego, S. S. Taylor (University of California, San Diego) and H. E. Hamm (Vanderbilt University).

The STS is able to bridge these gaps and will allow neutrons to be used in a transformative way to unify the structural and dynamical description of biological systems across length and time scales. This advancement will transition the concept of a predictive understanding of biological systems to a reality.

2.1.4 Materials Discovery, Characterization, and Application[5]

Materials are at the heart of technologies that will define the future economy and provide solutions to the challenges in energy, security, and transportation. Predictive modeling of materials holds the promise of accelerating the development of new solutions; however, as a prerequisite, this development requires an understanding of materials' structure and dynamics from the atomic scale to real world components and systems. In addition, understanding and modeling synthesis and processing are vital to achieving transformative impact.

The unique physical properties of neutrons make high intensity beams indispensable to materials discovery, characterization, and application where they complement the capabilities of electrons and photons. Among these characteristics, their nondestructive nature, ability to penetrate real components and materials under working condition, sensitivity to light elements, ability to observe modes and dynamics over virtually all length and time scales, absence of selection rules, and the ability to highlight components using isotope substitution make their contribution unique. Areas where neutrons will be essential for future materials science and engineering include infrastructure stewardship, advanced propulsion systems, advanced materials processing, nuclear fuels and radiation tolerant materials, energy storage and energy conversion integrated systems, materials by design (integrated computational materials engineering), and materials under extreme environments.

To meet future challenges, new developments are needed in the following:

- Monitoring and understanding chemical reactions and catalysis including gas adsorption and separation.
- Using analytical chemical spectroscopy where neutrons could provide a high throughput technique, providing information not accessible to photons.
- Understanding the role of disorder and defects and learning how to manipulate.
- Addressing the fundamental challenges of glasses and liquids as well as fluid flow and reactivity.
- Conducting *in situ* studies under pumping conditions, kinetics studies, materials growth and synthesis, and materials under extreme conditions.
- Understanding how components and integrated materials in devices function under realistic conditions using instruments that can combine multiple techniques such as imaging, diffraction and spectroscopy.

The combination of intensity, dynamic range, and beam focusing at STS is crucial to provide transformative capabilities to enable these developments.

Overall, the outstanding scope of the science and technological challenges where neutrons play an irreplaceable role ensure they will be needed as a central part of a national facilities strategy for decades

[5] Report from "Frontiers in Materials Discover, Characterization, and Application" Workshop August 2–3, 2014, Schaumburg, IL, G. W. Crabtree (Argonne National Laboratory) and J. B. Parise (Stony Brook University).

to come and show the compelling need for forefront facilities to ensure scientific and technological competitiveness.

2.2 ADDRESSING FUTURE SCIENCE CHALLENGES WITH THE SECOND TARGET STATION

To connect these science challenges with the source capabilities provided by STS and determine how this would be complemented by the FTS and HFIR, 14 working groups were established that involved 70 NScD scientists. They were charged with exploring new concepts and instrumentation. Appendix 4 describes concepts for 19 neutron scattering instruments developed by these teams and three additional concepts submitted for consideration as part of this workshop. Gains in performance of two orders of magnitude and beyond over existing capabilities make it transformative for many of the compelling research areas identified. At the heart of this dramatic step forward in capabilities are a series of advances that, when combined, create new classes of instrumentation. The major drivers for this advancement include the advances in target and moderator technology, as well as high performance computing that enables reconstruction and analysis of multimodal data and simulation of systems gluing together disparate data sets and open complex scenarios to analysis and interpretation. In addition, advances in manipulation of the spin of electrons, nuclei, and neutrons allow control of scattering cross sections and contrast *in situ* and revolutionize what can be measured in magnetic and hydrogenous materials.[1] Another area of great advance is in neutron optics where lensing, guiding, and wavelength analysis are all taking major steps forward. Taken together, these define STS as a new generation of neutron facility of far reaching science impact.

Overall, development of the STS will ensure the United States leads in neutron sciences for the foreseeable future. It will impact our understanding of materials by giving an integrated understanding from the atomic to real world scales. It will provide unprecedented access to mesoscale quantum and complex matter and ensure that the unique contributions of neutrons to discovery and understanding in these fields continue for decades ahead. The advent of 3D mapping and micro-spot technologies as well as the source intensity and novel instrumentation allow *in situ* and *in operando* studies, not just of exemplary materials but also of real operating systems, in the most challenging problems in technology and engineering. Automation and high throughput instrumentation, coupled with advanced modeling, databases and libraries, will put STS center stage coupling big data with computational resources to enable predictive control and design of materials. Already, the close relation between theory and experiment is putting neutrons at the forefront of the revolution in combining simulation and data. The high intensity beams and advanced handling capabilities will bring new insights into kinetics, out of equilibrium, and chemical reactions. They will facilitate not just the understanding of materials but also their synthesis and impact of processing conditions. Such capabilities will become all the more important as the prediction of compelling material compositions makes advances in their synthesis all the more pressing. Finally, the major step forward in capabilities possible with STS will reach out into new science areas and bring whole areas of science, like biology and materials chemistry, into reach where the unique properties of neutrons can then play as important a role as they do today for quantum condensed matter and soft materials.

3. SCIENCE DISCUSSION WORKING GROUP SUMMARIES

This section contains reports from the focus groups, which centered on the scientific case for the STS. Based on the conclusions of the Grand Challenge workshops, the groups discussed important scientific opportunities that should be addressed over the next decade and how the STS will benefit these opportunities. The following reports were prepared by the discussion chairs.

3.1 MEMBRANES AND THIN FILMS

David Worcester (chair), National Institute for Standards and Technology Center for Neutron Research/University of Missouri (emeritus); William Heller, ORNL; Rex Hjelm, Los Alamos National Laboratory; John Katsaras, ORNL; Jaroslaw Majewski, Los Alamos National Laboratory; Eugene Mamontov, ORNL; Shuo Qian, ORNL; Greg Smith, ORNL

The Membranes and Thin Films working group addressed the uses of neutron scattering for studies in two science areas: biological membranes and non-biological thin films also including biomimetics. The scientific opportunities in these two areas are rather different and are addressed separately below. However, the experimental needs of these two areas are quite similar, so the latter part of the summary does not distinguish between the two areas. The Membranes and Thin Films working group shares much with both the Biology and the Soft Matter working group.

Scientific Opportunities

Scientific opportunities in biological membranes research are growing rapidly and this can be expected to continue for many decades. Membrane proteins constitute about 30% of the proteins in a cell and perform many of the cell's most important functions, affecting issues of health and development in humans. Structures and dynamics of such proteins and their complexes are vital to understanding the mechanisms of these functions. However, protein crystallography has only recently begun to be significantly successful in providing structural information for membrane proteins and their complexes. This is largely due to the difficulties of purifying and crystallizing membrane proteins. Compared to the wealth of crystal structures for water-soluble proteins, membrane proteins are behind. As a result, membrane protein research has been a priority area for National Institutes of Health funding the past 10 years. This included methods that do not rely on crystals for structural information and has provided many important successes, some of them quite spectacular. But there is still a great amount of work to do, especially in the very important general area of cell signaling pathways, which includes the ion- and membrane-based electrical signaling of nerve cells. Details of protein interactions within membranes and on membrane surfaces are key aspects of many cell signaling pathways, especially for the very large family of G-protein coupled receptors. New technologies to enable this work are an important focus of attention.

Neutron scattering methods have been used to study biological membranes for more than four decades and have contributed much, especially to the understanding of structure and dynamics of bilayer model membranes and more recently membranes that include particular proteins. A variety of neutron scattering techniques are currently used to study membranes, which are often prepared in a variety of different ways. Improvements in these neutron techniques, especially in regard to rate of data collection, will provide important benefits.

Neutron reflectometry has been used extensively, especially with the development of tethered membranes and flow cells for the study of single membranes in a fully hydrated environment close to natural conditions and in which components and conditions can be readily changed, including for kinetic studies. Conditions that can be changed with tethered membranes now include a voltage across the membrane, which is an important aspect of cell membranes and regulates the activities of many membrane proteins.

Neutron diffraction from multilayers of membranes was the earliest method of neutron scattering studies and is still being used for structural work due to the advantage of obtaining data to higher Q than reflectivity from single membranes, usually by a factor of two. Deuterium techniques are the method of choice for solving the phase problem.

Neutron crystallography of membrane proteins is also important but is more limited due to difficulties of obtaining crystals of suitable size and the very long times needed for data collection. Nevertheless, such

work offers unique opportunities using hydrogen/deuterium changes for elucidating important roles of disordered water and lipids in the function of membrane proteins, especially ion channels. It can locate disordered parts of proteins not visible in x-ray crystal structures. It is also possible to determine special hydrogen bonding arrangements that are not determined by x-ray structures.

Vesicles of membranes dispersed in water are extensively studied by neutron small-angle scattering. There is much work in this area because of the unique opportunities provided by contrast variation techniques and selective deuteration.

Neutron spin echo (NSE) has become very useful for clarifying special aspects of membrane dynamics, especially in determining bending moduli and how they change with composition and other conditions. Membrane thickness fluctuations have also been elucidated by NSE studies.

All of these methods are expected to be important for the study of membranes for decades to come. As the studies increasingly address aspects of membrane proteins that are difficult to produce and purify, neutron facilities capable of studying small samples will be needed. In addition, selective deuteration of components will provide the unique advantages and opportunities of neutron scattering studies.

Developments in fabrication of thin polymer films now include incorporation of colloidal particles of diverse size, shape and chemistry. In addition, nanoscale arrangements of components can be kinetically trapped or adjusted by annealing, providing altogether a large parameter space for samples. Energy storage and purification technologies and sensor technologies are among the areas that will benefit from these new materials. Specular neutron reflectometry is an important depth-profiling technique for characterizing the nanoscale structure from sub nanometer to the order of a 0.1 μm of such materials over lateral length scales of many microns to millimeters, without damage to the soft material and with the unique advantage of altering contrast with deuterium. However, instrumentation will be needed for studying small samples, which is the key parameter for most future work.

Other examples of scientific opportunities in thin films include catalytic and redox reactions at catalyst/polymer interfaces, polymer organization at interfaces and voltage cycle hysteresis, filtration membranes and *in situ* dynamic responses of polymers at interfaces, to name just a few. An advanced reflectometer with significantly better intensity and lower background is required to fully characterize these materials. Furthermore, higher intensity with advanced data acquisition systems will enable kinetic studies, particularly for the study of molecular level responses responsible for the characteristic cyclic states of these materials using stroboscopic, pulsed-probe techniques.

Benefits of STS

The main enabling characteristic of the STS for studies of thin films and biological membranes will be enhanced reflectometry capability. Higher intensities, more rapid data collection due to large wavelength bandwidth with lower relative backgrounds will provide the capability to measure smaller samples, to do kinetic studies including pulse-probe measurements, or to study interfaces under conditions that cause structures to be stable only over shorter time scales. Improvements in resolution, especially off-specular, will also be a benefit.

Small and wide angle membrane diffraction, including from single crystals of membrane proteins will benefit from STS primarily by enabling measurements of smaller samples and obtaining data simultaneously in large regions of reciprocal space. The large Q range available to some instruments is needed for this work. For crystals of membrane proteins, reducing the minimum crystal volume by one order of magnitude from the requirements of current instruments, such as SNS BL-11B, MaNDi, is needed to measure crystals of the size currently available for many membrane proteins. Further reduction of required crystal volume would be a very significant bonus.

For membrane dynamics, STS will provide capability in back-scattering spectroscopy that will overlap considerably with spin echo spectroscopy. This will enable measurements of diffusion processes as well as measurements of membrane flex dynamics that were previously only possible with spin-echo spectroscopy.

STS to complement FTS and HFIR

For studies of thin films and biological membranes, the STS will be an improvement over the FTS, primarily from the larger wavelength bandwidth but also moderator optimization and beam technologies that enhance intensity over the required wavelength domain and lower relative backgrounds. Complementarity arises primarily with HFIR and STS, as SANS and spin echo spectroscopy instruments have significant domains of experimental approach at these sources where they perform best. HFIR SANS capability will be especially needed for measurements of vesicle systems, including protein-membrane interactions and for the in-plane structure of other membranous materials. HFIR NSE spectroscopy will be an essential complement to STS backscattering spectroscopy for membrane flexing and bending modulus measurements. For softer membrane fluctuations such as membrane thickness fluctuations, HFIR spin echo spectroscopy capability will be essential.

Complementary Experimental Techniques

Foremost among complementary techniques is the need to better manipulate contrast and highlight special components by deuteration. Increased support is needed for biological deuteration, especially for deuteration of membrane proteins and purifying them, since these are often especially difficult processes. Segmental labeling methods permit linking two polypeptide chains with different isotopic compositions. So far this method has been limited to a few specialized laboratories for segmental labeling for nuclear magnetic resonance (NMR). Its more general application to neutron scattering could have significant benefits. New technical developments in this area could make application for neutrons more routine. Likewise, support for chemical deuteration, particularly for polymers is essential to fully utilize contrast control in membranous materials.

For reflectometry studies of tethered membranes in flow cells, sample environments for pulsed probe measurements, a wet chemistry laboratory at the instrument is needed since changes of flow solutions will be frequent. Capabilities of a laboratory on a beam line, such as ultraviolet (UV) and visible spectroscopy for concentration measurements and circular dichroism for protein secondary structure evaluation will also be important. For thin films, *in situ* processing will be desirable.

Auxiliary Requirements

Sample environment needs for studies of thin films and biological membranes are not very demanding since extreme conditions are rarely needed. Basic needs include the following:

Temperature control from 5 to 50 °C for biology
Somewhat higher temperatures for thin films
Hydrostatic pressure cells to 2 kbar
Humidity cells for frequent humidity changes by electronic control
Humidity cells for high humidities near bulk water hydration
Electric field application and control to tethered membranes
Magnetic fields of at least 2 or 3 Tesla (T)
Shear fields for rheological studies
Pulse/probe instrumentation and data acquisition for this mode

In addition, theoretical analysis and data analysis software development is needed for application of the Distorted Wave Born Approximation to off-specular reflectometry.

Instrument Priorities for STS
The membranes and thin films session quickly converged on the following instruments to recommend for early construction at STS:

1) QIKR for reflectometry.
2) SWANS for multilayer diffraction and "medium-Q" SANS studies, but suggest an option of reduced minimum Q from the current 0.01 $Å^{-1}$ by at least a factor of two, and accepting a related reduction of Q_{max}.
3) EWALD/DYPol dynamic nuclear polarization (DNP) for crystal structures of membrane proteins. This instrument and DNP technique are likely to be "game changers" for neutron protein crystallography, including membrane proteins.
4) MBARS for μeV backscattering measurements, for studies of molecular diffusion in membranes and membrane flexing dynamics.

Low-Q SANS and NSE measurements are best done at HFIR and should be strongly supported for work on membranes and thin films.

3.2 STRUCTURE AND DYNAMICS OF BIOMACROMOLECULES, LARGE COMPLEXES, AND INTRINSICALLY DISORDERED SYSTEMS

David Cowburn (chair), Albert Einstein College of Medicine; David Banks, University of Tennessee; Annette Bodenheimer, North Carolina State University; Julian Chen, Los Alamos National Laboratory; Leighton Coates, ORNL; Matthew Cuneo, ORNL; Oksana Gerlits, ORNL; Gnana Gnanakaran, Los Alamos National Laboratory; Zhen Huang, Georgia State University; Choel Kim, Baylor College of Medicine; Andrey Kovalevsky, ORNL; Joanna Krueger, University of North Carolina, Charlotte; Susan Krueger, National Institute for Standards and Technology; Flora Meilleur, ORNL/North Carlonia State University; Diana Mitrea, St. Jude Children's Research Hospital; Brad O'Dell, North Carolina State University/ORNL; Hugh O'Neill, ORNL; Marc Pusey, iXpressGenes, Inc.; Lee Robertson, ORNL; Don Ronning, University of Toledo; Venu Vandavasi, ORNL; Kevin Weiss, ORNL; Qiu Zhang, ORNL

Scientific Opportunities
There is a long history of promise of neutron methods in structural biology, but the broad impact of the methods has been limited by both insensitivity of detection, and limited opportunities for access by structural biologists. Both issues are addressable by the proposed STS. Of particular note, macromolecular neutron crystallography provides accurate positions of hydrogen atoms vital to elucidating the mechanism of enzyme action, and the selective binding of ligands including optimization of potential therapeutics' design.

SANS provides shape and scale information on biomolecular complexes, permitting selective measurements on isotopically manipulated portions augmenting their structure characterization. This is of special significance for intrinsically disordered proteins and regions of proteins, where their interaction mechanisms are generally unknown. Such investigations can provide unique insights into physiological and pathological processes, including amyloid formations, and function of pores, non-membranous assembly processes and cytoskeletal elements. This area overlaps soft matter investigations of biological materials.

Neutron methods have a unique role in potential contributions to calibrating time dependent processes needed for spatio-temporal simulation of large-scale biological structures. The nano-microsecond range of

motions is particularly in need of such experimental methods, and spin echo and similar developments have the unique potential to provide critical data in this range.

New neutron instruments can then contribute to both new transformational science in structural biology, in addition to its existing recognized role as part of integrative structural biology.

Benefits of STS
Currently, a large number of potential users are deterred by the long wait for beam time, and the triage of reviews which result from the lack of resources both for crystallography and for SANS. Any increase in available resources is of importance, in addition to the unique scientific capabilities of new STS resources.

New diffraction resources in STS can provide unique opportunities for macromolecular crystallography. The novel development of DNP has the potential to be a major transformational event for neutron crystallography. Significant technical progress towards a prototype was presented. Other STS resources can relieve demand on HFIR beam lines providing additional user availability for SANS methods.

STS to complement FTS and HFIR
For SANS, current and augmented HFIR beams provide high flux, which is the principal limitation for many biomolecular applications. However, an increase in available beam lines for SANS will be of great significance in increasing capacity to deal with demand, and STS SANS will provide suitable capabilities for the class of experiments with larger coherent scattering (e. g. protein complexes > 250 kDa, membrane systems, etc.).

Complementary Experimental Techniques
ORNL has a good history of providing near beam line wet laboratory space and this should be continued. Additional sample prep (re-prep) might include liquid chromatography, multiangle light scattering detection, etc.

The use of contrast variation by isotopic manipulation, principally deuteration, can be a major deterrent to new users. Local expertise in new developments in segmental and site specific labeling would be of major aid to many potential investigators.

Auxiliary Requirements
The sample environment issues are similar to those described for membrane systems above and so are not repeated. With regard to software, there is a general opportunity to develop more precise collective variables for levels of course spatio-temporal modeling associated with bio- and other soft materials across the board. High quality simulation provides insights and design of new experimental approaches critical to both the biomolecular and general materials research.

The general availability and high quality documentation of data reduction and first order analysis of course remains a major objective for user support.

3.3 COLLOIDS, SELF-ASSEMBLED SURFACTANTS, CHARGED POLYMERS IN SOLUTION, POLYMER NETWORKS, HYDROGELS, NANOCOMPOSITES AND HIERARCHICAL SYSTEMS

Tonya Kuhl (chair), University of California, Davis; Sudipta Gupta, University of Tennessee, Knoxville; Yuri Melnichenko, ORNL; Philip Pincus, University of California, Santa Barbara; Yin Panchao, ORNL

Science Opportunities
The STS will enable significant advances in soft matter research through advances in instrumentation and beam flux which will permit dramatically shorter measurement times, larger accessible Q ranges, and highly focused (small) beams on sample. To fully take advantage of the capabilities of STS, soft matter research requires complementary characterization and *in situ* auxiliary environments to study structure in dynamic environments including control over temperature, pressure, shear, and applied fields (e.g. electric, magnetic, chemical, etc.).

Benefits of STS
Soft matter systems and hybrid soft/hard composite materials are frequently systems with numerous local energy states with different properties and structures. The science enabled by STS with soft matter is very broad, from how to improve the properties and functionality in hybrid soft/hard composites and active soft materials, design interfaces with defined structures and functions, drive weakly ordered systems to specific states with high uniformity, to complex structures in solution and hierarchical assemblies. Specific examples that should become possible with STS include directly measuring – transition states as a protein unfolds, ion transport and the structure of a cathode while a battery is operating, to general changes in molecular structure and electronic states under working conditions to reactions to studying and characterizing fluctuation modes that become dominate as a system approaches a transition state. To study and characterize soft matter systems requires *in operando* conditions, highly selective deuteration, numerous complementary techniques, ultra-advanced data modeling, and coordinated computer simulations.

STS to complement FTS and HFIR
Opportunities to optimize between STS, FTS, and HFIR are well developed. A critical need for soft matter research is sophisticated fabrication methods and secondary characterization capabilities co-located with these facilities. In short, soft matter systems must frequently be studied shortly after fabrication or even during fabrication and the same sample must have multiple characterization methods. STS and upgrades to SNS and HFIR offer the ability to design and optimize instruments to truly integrate multiple techniques to characterize a single sample on multiple length and time scales under controlled environmental or working conditions. Moreover, co-refinement of multiple data sources to extract the most comprehensive information on a sample is enormously limited by not being able to do simultaneous characterization on a single sample. Improved integration and flexibility to meet user needs from fabrication to measurement capabilities are necessary to take full advantage of the opportunities of these facilities.

Auxiliary Requirements
Beyond physical hardware and infrastructure, the soft matter community needs improved analysis software and collaboration with modeling and simulation experts as part of the instrument package to handle complicated, real samples of today and tomorrow. The community and science has reached a point where being able to analyze neutron scattering data in novel and sophisticated ways precludes broad user participation and may potentially limit the science that can be done.

3.4 DYNAMICS IN SOFT MATTER, GLASSES, GELS, TRANSPORT IN SOFT MATTER, AND ACTIVE SOFT MATTER

Yun Liu (chair), National Institute for Standards and Technology Center for Neutron Research/University of Delaware; Lowell Crow, ORNL; Wei-Ren Chen, ORNL; Changwoo Do, ORNL; Takeshi Egami, ORNL/University of Tennessee; Jun Han, ORNL; Youngkyu Han, ORNL; Luke Heroux, ORNL; Kenneth Herwig, ORNL; Luis Sanchez Diaz, ORNL; Gerald Schneider, Louisiana State University; Yangyang Wang, ORNL; Zhe Wang, ORNL; Yang Zhang, University of Illinois, Urbana-Champaign;

Scientific Opportunities

Soft matter research encompasses a wide variety of materials important for both academic fields and industrial applications, including the pharmaceutical, petroleum and cosmetic industries as well as manufacturing and chemical processing. Many soft matter materials have very complex structures that need to be characterized from nanometers to millimeters. This broad range of length scales is typically associated with dynamics occurring over an even wider range of time scales making the study of soft matter dynamics particularly challenging, perhaps even more so than the structural characterization. Many soft matter systems have a hierarchical structure resulting in more complicated hierarchical dynamics. Examples include highly stretchable hydrogen gels and polymer composites, whose dynamics can easily span through many orders of magnitudes in the time scale. Neutron scattering techniques have historically provided and will continue providing unique insights into soft matter dynamics. Discussions in this breakout session identified the following research directions as examples that require the development of new neutron scattering measurement capabilities.

Dynamics of bio-membrane based systems: There is increasing interest in the behavior of complex biological systems and the dynamics of biomimetic macromolecules under different working conditions. Examples include membrane fluctuations and lateral motions of membrane proteins and membrane domains. Even though neutron scattering techniques can access the time and length scales characteristic of these motions, continued progress relies on higher availability and better performance of new instruments, such as NSE instruments optimized for large-length and long-time scales, and higher resolution backscattering spectrometers with large dynamic range.

Slow dynamics of proteins/small biomolecules in concentrated solutions and crowded conditions: The behavior of biomolecules in crowded solutions is of interest both for industrial applications and understanding the influence of "real-world" operating conditions. For example, recent development of subcutaneous injection methods of fast growing monoclonal antibody based therapeutics requires the development of protein formulations at very high concentrations. However, protein motions are significantly slowed down when the concentration increases. Hence, the development of instruments that can access long correlation times is highly desirable.

Internal dynamics of protein and polymeric systems: The study of internal dynamics of complex materials including protein domain motions and segment dynamics of polymeric systems have been identified as important research directions. The capability of measuring the dynamics at different length scales by neutron scattering techniques provides unique opportunities for the soft matter community to interrogate the dynamics of internal structures. While there have been an increasing number of such studies, community growth in this field has been seriously limited by the available neutron beam time for instruments suitable for this study.

Gelation and glass transitions: Studying liquid-solid transitions, especially glass transitions, has long been a scientifically active, yet very challenging topic. Glass transitions can be found in many different systems, such as metallic systems, glass forming molecular liquids, protein/colloidal dispersions, and polymeric systems. Its fundamental understanding has a far-reaching impact to many important fields. Investigations of both the beta-relaxation and alpha-relaxation times are critically important to elucidate the physical mechanisms of glass transitions. However, the time scale for beta-relaxation and alpha-relaxation can differ by many orders of magnitudes. For example, the study of metallic glasses requires the capability to access the dynamics from picosecond to minutes with the sample temperature over 1000 ˚C. Study of a protein/colloidal system requires a capability to access dynamics on time scales ranging from a few nanoseconds to days at the length scale comparable to particle size. Given the large time scale difference of systems, a range of instruments are needed with the capability to access large dynamic ranges.

Structural and dynamic changes under external stimuli: Complex fluids can be found in many applications including colloidal solutions, paints, shampoos, pharmaceutic products, and batteries. The structure and dynamics of complex fluids have long been studied by various neutron scattering techniques. Recent interest has focused on the structural and dynamic responses of complex fluids to external stimuli including shearing forces, pressure, temperature, pH value, and electric/magnetic fields. This class of materials promises control and/or adaptation of functionality matched to individual applications. Investigation of both structural and dynamic changes in response to stimuli is critical to elucidate the fundamental physics mechanisms underlying this behavior. Instruments that enable study of samples under a variety of external fields with good spatial resolution that support stroboscopic methods are needed.

Benefits of STS

The high neutron brightness of the STS makes it possible to use much smaller sample volume, opening the window for new science that has long been limited due to the scarcity of samples such as some biological materials and bottom-up designed novel nanomaterials. The slow repetition frequency at the STS allows development of new types of instruments providing unique dynamics windows that are currently challenging to access.

Because of the large range of time scales needed to study soft matter dynamics, it is important to develop a suite of instruments that can cover as wide range of dynamic windows as possible. For example, the proposed MBARS instrument can extend the current capability of backscattering techniques to study even smaller Q value (larger length scale) with improved energy resolution, and the discussed BWAVES instrument can offer the capability of measuring a wide range of dynamics in a single instrument. These instruments will also complement the existing instruments or future instruments at HFIR and FTS.

STS complement to FTS and HFIR

Based on the three neutron source strategy at ORNL, it is important to point out that the high resolution NSE instrument is better developed at HFIR to enable the study of slow dynamics. This NSE can complement the instruments developed at STS and FTS to provide correlation time from a few picoseconds to more than 100 nanoseconds using long neutron wavelengths from 13 Å to 17 Å. This type of instrument is essential for studying protein solutions, polymer melts, and polymer/polyelectrolyte solutions. For this purpose, a dedicated cold source for a neutron spin echo with the capability to provide these long wavelength neutrons would provide U.S. researchers access to long correlation times with unprecedented flux and extremely low backgrounds.

Auxiliary Requirements

A good user interface for the instrument control/operation and sample changes is essential for users to make optimal use of the beam time.

There is a need to upgrade existing and develop new sample environment equipment to meet the needs of the community to perform cutting-edge experiments. Examples include the development of the *in situ* shearing cells, microfluidic flow cells, high temperature ovens, and sample cells with large external oscillatory magnetic or electric fields.

Polarization techniques would be useful to help separate the coherent motions from the incoherent motions and resolve structural features with unparalleled details when both coherent and incoherent scattering contribute significantly to scattering signals. Selective deuteration support to the community for preparing high quality samples is critically important for detailed study of both the structure and dynamics of targeted components of complex systems. The development of computational tools and theoretical models is essential to analyze and interpret scattering data from complex systems.

3.5 HETERO- AND NANO-STRUCTURED MATERIALS

Charles Majkrzak (chair), National Institute for Standards and Technology Center for Neutron Research; Haile Ambaye, ORNL; Katie Andrews, ORNL; Lisa DeBeer-Schmitt, ORNL; Morten Eskildsen, University of Notre Dame; Michael Fitzsimmons, ORNL; Boris Khaykovich, Massachusetts Institute of Technology; Valeria Lauter, ORNL; Honyung Lee, ORNL; Chris Leighton, University of Minnesota; Yaohua Liu, ORNL; Eric Lukosi, University of Tennessee; Steve May, Drexel University

Scientific Opportunities

The working group began by discussing at what length and time scales, in general, does the research community want to be able to measure the scattering of neutrons by hetero- and nano-structured materials. The group concluded that being able to image the variation of the nuclear or magnetic scattering length density (SLD) from 1nm or one unit cell length to 10 microns and study kinetic (time-dependent) perturbations of electric and magnetic fields over 1s to 1 microsecond. In particular, it would be of interest to perform stroboscopic measurements at a time scale of 0.1 ms and to be able to do micro-diffraction (micro meaning over a 1 to 10 micron region).

Some examples of scientific problems to be investigated include superconductor vortex structures and magnetic domains within bulk materials — with resolution ranging from that of SANS to imaging (i.e., from 100 nm to 100 microns). There is a need to see the interior volume of the bulk as opposed to the surface region (which is probed optically or, for example, by spin-polarized low energy electron diffraction [SPLEED]).

In addition to structure determination, the working group determine it would valuable to study excitations in 100 Å thick films (i.e., the order of several hundred micrograms would likely be needed), at interfaces, and within confined structures. But resonant inelastic x-ray scattering (RIXS) techniques at higher energy transfers are steadily advancing, so neutron scattering methods should be focused on lower energies — such as needed in studies of confined and mesoscale thin film systems (10 meV to neV). For example, skyrmion vortices are larger scale structures so excitations (coherent and incoherent) are lower energy. New neutron scattering instruments should focus on other excitations than phonons and spin waves.

Some of the specific scientific problems that pertain to hetero- and nano-structured materials that can be addressed with neutron scattering techniques include correlating fatigue with changes of structure, investigating ionic control of magnetism at liquid/solid interfaces, exploring systems in which a crossover occurs in going from stroboscopic (time domain) to dynamics/excitations (frequency domain), performing form factor measurements of thin films to obtain the unpaired electron distribution within a unit cell, determining spin structure across a domain wall, studying the dynamics of vortex matter versus current, and determining the variation of order parameter versus proximity to interfaces in comparison bulk behavior (via grazing angle diffraction).

In addition, the working group noted in many of the systems mentioned above, a holistic view can emerge by combining neutron scattering (over many length and time scales) with transport measurements.

Finally, the working group had some general comments regarding the application of neutron scattering as a probe of hetero- and nano-structured condensed matter systems: 1) it is important to extend the existing limits of wave vector transfer Q and minimum signal (reflectivity) to enable reflection and diffraction studies of ever thinner layers and interfacial regions (e.g., confinement of superconductivity, magnetism, etc., in thin films can result in very different behaviors than what is observed in bulk volumes); 2) nanoscale thin film structures can exhibit significant physical properties not only as a function of depth into a film but also of position in-plane as well, so it can be essential to be able to measure wavevector

transfers laterally and not just perpendicular to an interface (i.e., the ability to measure both specular and non-specular scattering is required; skyrmions, magnetic inhomogeneity in vortex systems); 3) neutrons should be used to probe hetero-structures where complementary to x-rays (e.g., soft resonant x-ray reflectivity); 4) large scale structures can have form factors that suppress scattering as Q gets larger, therefore demanding higher incident intensities and better signal to noise ratios -- the goal should be to isolate a signal produced by a 10 nm thick layer from scattering due to a substrate that is 1 mm thick at a 10^-8 reflectivity level (thus particular attention must be paid to minimizing background from sample environment and other external sources).

Benefits of STS

The STS enables measurements over broad ranges of length and time scales simultaneously — in systems that inherently may change with time. The low repetition rate of the STS means that it is possible to build long instruments to accommodate focusing without too much sacrifice of Q-band. The STS also enables "single shot" experiments covering a wide range of wave vector transfer Q simultaneously.

STS complement to FTS and HFIR

The STS allows optimization of a cold or very cold neutron source for instrumentation available at a green field site. Better resolution than what is available at HFIR, so the time of flight (TOF) gain works to advantage at the STS.

Complementary Experimental Techniques

Beam time must be spent in a known well-defined state. *In situ* diagnostics are necessary (e.g., transport, alternating current (AC) susceptibility, Magneto Optic Kerr Effect (MOKE), O_2 measurement, microwaves for magnetic resonance, etc.).

Computational modeling ideally performed in real time with the neutron scattering is imperative. Neutron scattering studies of bio-membrane systems done in conjunction with molecular dynamics simulations is a prime example. This requires collaboration with computational modelers and high-performance computing facilities.

Auxiliary Requirements

A considerable complement of auxiliary equipment and sample environments are required to perform the types of measurements discussed above. Sample environment control of magnetic fields (spin textures can be complicated phases affected by high magnetic fields >30T), electric fields, temperature (over a range from 50 mK to 1200 K -- to the melting points of refractory materials) and pressure are needed. The ability to perform *in situ* measurements such as transport, AC susceptibility, and MOKE are also required for certain experiments. Other potentially important equipment include gas and liquid handling systems, chemical environments, devices for cleaving crystals *in situ*, sources of light for use as "catalysts" to illuminate surfaces to change the polarization of ferroelectrics, and ion implantation devices for implementation on the beam line as well as ultra-high vacuum chambers to enable *in situ* cleaning of surfaces and subsequent physical and chemical vapor deposition. Software to effectively synchronize ancillary measurements with neutron detection also needs to be provided.

Capability for polarized incident neutron beams and polarization analysis of scattered neutrons are required along with an option for polarimetry utilizing a "cryocup" type device -- a zero-field magnetic environment. It would also be prudent to provide options for modulation techniques (stroboscopic, spin nutation, Larmor precession) to further enhance the efficiency and sensitivity of the instrument for certain types of measurements. A local laboratory environment for sample preparation would be another important addition.

To realize all of the above, it might be more efficient to embed sample support personnel in the instrument team. There may also be a need for additional specialized expertise to support sample environment. Finally, to successfully implement many of the ideas discussed may require a detailed simulation of a complete package from target to detector.

3.6 BULK FUNCTIONAL MATERIALS AND EMERGENT STATES OF MATTER

Raymond Osborn (co-chair), Argonne National Laboratory and Bruce Gaulin (co-chair), McMaster University; Douglas Abernathy, ORNL; Adam Aczel, ORNL; Stuart Calder, ORNL; Claudia Cantoni, ORNL; Huibo Cao, ORNL; Songxue Chi, ORNL; Andrew Christianson, ORNL; Pengcheng Dai, Rice University; Antonio dos Santos, ORNL; Georg Ehlers, ORNL; Jaime Fernandez-Baca, ORNL; David Freeman, ORNL; Ovidiu Garlea, ORNL; Garrett Granroth, ORNL; Sara Haravifard, Duke University; Tao Hong, ORNL; Marc Janoschek, Los Alamos National Laboratory; Young-June Kim, University of Toronto; Stephen Kuhn, University of Notre Dame; Hans Jochen Lauter; Seunghun Lee, University of Virginia; Jonathan Leiner, ORNL; Jiao Lin, ORNL; Mark Lumsden, ORNL; Masaak Matsuda, ORNL; Rob McQueeney, Iowa State University; Martin Mourigal, Georgia Institute of Technology; Stephen Nagler, ORNL; Stephan Rosenkranz, Argonne National Laboratory; Andrei Savici, ORNL; Matthew Stone, ORNL; David Tam, Rice University; Wei Tian, ORNL; John Tranquada, Brookhaven National Laboratory; Bogdan Vacaliuc, ORNL; Jinchen Wang, University of Kentucky; Meng Wang, University of California, Berkeley; Travis Williams, ORNL; Barry Winn, ORNL; Ming Yi, University of California, Berkeley; Igor Zaliznyak, Brookhaven National Labortory

Scientific Opportunities

The working group identified five broad areas of materials science in which the new cold neutron capabilities at STS could lead to great advances. All of these areas correspond to the identification of new states of matter and a microscopic understanding of the ingredients that lead to such states, such that they can be quantitatively predicted, created and manipulated. The working group also discussed specific topical questions for which we hope uncover definitive answers.

1. Quantum Magnetism: Can a quantum spin liquid in greater than one dimension be realized? Can entanglement entropy in bulk matter be measured?
2. Unconventional superconductivity: Can room temperature superconductivity be achieved? How universal is unconventional superconductivity? Can the competing orders that often accompany unconventional superconductivity be understood?
3. Quantum critical phenomena: Can clean quantum criticality be observed?
4. Itinerant magnetism: Can a 100% spin polarized conductor be realized? Can a room temperature insulating ferromagnet for spintronic applications be realized? How does charge transport relate to magnetic order?
5. Topological Materials: Can the topologically-protected band structure of a Weyl or Dirac semi-metal be probed? Are there novel topological quantum phases in materials with large spin-orbit coupling?

The working group discussed the specifics of how the STS would enable the scientific advances described above. These are predicated on several characteristics of the STS and the new instrumentation that will be developed for it.

The time-structure of the STS implies that it will be very well suited for cold neutron applications, and these are in great current demand at the FTS. For example, SNS BL-5, CNCS, is currently handling the cold chopper spectrometer demands at SNS and it is typically oversubscribed by factors of 4-5 during

each beam time competition cycle. Such a strong oversubscription factor is sufficient to curtail and stop compelling beam time proposals for such cold neutron spectroscopic applications, and discourage the relevant principal investigator (PI) from continuing further in this area of research. So, there is a prima facie case for much better access to infrastructure for cold neutron inelastic capabilities at SNS.

As many of these applications are associated with the studies of new materials, such cold chopper spectrometer projects often employ relatively small single crystals, as are typically available at the beginning of a research field. Therefore, infrastructure that has been optimized for the study of small single crystals are likely to find great influence in the science which is of interest.

Such high brightness sources and instrumentation will also open up opportunities for very novel neutron scattering studies. These include spatial mapping of the scattered intensity to study inhomogeneity on an appropriate scale, and relatively easy integration with spatially-confining sophisticated sample environments, such as high pressure experiments.

It will be important be integrate all new design features into the new instrumentation at STS, such that the enhanced flux of low energy neutrons is used as efficiently as possible and elucidates structure and dynamics over as wide a dynamic range as possible. This includes the efficient use of sample changers (such as low temperature carousels, at least for powder samples), continuous sample rotation capabilities and the efficient use of multi-rep-rate methods such that the most information possible can be extracted from a single experiment.

The gold standard for the type of INS experiment that will address the new science being targeted is full polarization analysis of S(Q, E) as a function of sample environment. Great advances have been made which will allow S(Q, E) to be efficiently measured over a large dynamic range in Q and E, but polarization analysis coupled with large position-sensitive area detectors typical of chopper spectrometers remains a challenge. Nonetheless, such detailed information would allow great progress related to new materials, and should be vigorously pursued and integrated into the new instrumentation at the STS.

The use of multi-rep-rate techniques and efficient Q-E mapping of the scattered neutron intensity, perhaps with polarization analysis will translate into very large data sets which will require efficient handling, manipulation, and analysis. Such manipulation of the big data sets will be needed on two time scales: one corresponding to hours, such that decision making and planning can occur at the experiment, and a more sophisticated manipulation such that exciting science is extracted, analyzed and presented for discussion and presentation. These requirements will place great demands on the ability to manipulate and other handle such large data sets.

Auxiliary Requirements

Sophisticated sample environment is sufficiently crucial to addressing the stated science goals with STS that it should not be considered as ancillary equipment, but should be considered an integral part of the instrument, for which key expertise must reside at STS from day one. Extremes of temperature, magnetic field, and pressure will allow novel phase diagrams with exotic phases of matter to be revealed by our neutron scattering experiments at STS. Constraints on the sample environments, such as on maximum magnetic field due to stray field pollution requirements, must be very carefully considered, as these will directly impact on scientific performance.

3.7 *IN SITU* CHEMICAL REACTIONS AND CATALYSTS

Thomas Hansen (chair), Institut Laue Langevin; Mark Bowden, Pacific Northwest National Laboratory; Chris Chapman, Georgia Institute of Technology; Yongqiang Cheng, ORNL; Luke Daemen, ORNL; Lawrence Falvello, University of Zaragoza; Chad Gillis, ORNL; John Gordon, Los Alamos National Laboratory; Thomas Huegle, ORNL; Ilia Ivanov, ORNL; Erik Iverson, ORNL; John Larese, University of Tennessee, Knoxville; Kuo Li, Center for High Pressure Science and Technology Advanced Research; Liyuan Liang, ORNL; James Neilson, Colorado State University; Daniel Olds, ORNL; Katharine Page, ORNL; John Parise, Stony Brook University; Timmy Ramirez-Cuesta, ORNL; Nancy Ross, Virginia Tech; Pamela Whitfield, ORNL; Robert Williams, Los Alamos National Laboratory; Zili Wu, ORNL; Haiyan Zheng, Center for High Pressure Science and Technology Advanced Research

Scientific Opportunities

A new challenge to approach in the field of investigating chemical reactions *in situ* by neutron scattering methods is to link structure and dynamics, to fulfill the Nobel Prize lecture promise of Brockhouse and Shull, having neutrons revealing where atoms are and what they do, also in the course of a chemical reaction. TOF neutron instrumentation such as available at the STS will be particularly well suited to this purpose as the simultaneous conduction of a diffraction experiment with sufficient reciprocal space coverage and resolution and spectroscopy is rather straightforward.

Multimodal approaches will be particularly helpful here, and proposed instruments like SWANS, SPHINXS, XTREME-X move the community forward. SNS BL-16B, VISION, is already used in this way.

A special interest is on the role of order and disorder also in reactions, a situation in which the precise quantitative observation of diffuse scattering along with the Bragg peaks is crucial. These total scattering experiments on evolving systems could be called dynamic pair distribution function (PDF), where one could, on top of what is exploited today, exploit the energy-dependence of the scattering (S of Q and ω).

Another special interest, especially when it comes to catalysis processes, is the observation of surface processes, of absorption and desorption. Physisorption is today routinely studied by diffraction methods, but the time dependence, as necessary for the understanding of catalytic processes, still mostly escapes the scopes of the currently available instrumentation.

When it comes to real time-resolution, a key parameter for the *in situ* study of chemical processes, the community is aware of some physical limits which are not likely to be overcome. Yet, there seems currently no need to overcome these, as on the other side of this "mirror" of time-scales one finds the panoply of spectroscopic methods. The later (spin-echo in particular) reach today out to above a microsecond, while the physical limit for "real" time resolution is about 10 microseconds This limit is set by the time required for a neutron to travel through a sample of finite size, as well as the detection gap of a neutron convertor. For reasons of intensity it will still be difficult to come close to this limit (stroboscopic methods or stop-flow methods will be needed), but one can expect time resolutions in the millisecond-range (i.e., the time needed to collect an exploitable diffraction pattern) to be obtained more routinely.

Examples for materials and processes of interest are the behavior of gases in clathrates, zeolites, metal-organic frameworks and other nano- and microporous materials, especially having in mind CO_2 sequestration and many other energy economy relevant processes, surface processes, to mention an exotic one, the ortho-para conversion of hydrogen, mineralization processes, proton and small-molecule transport and other reactions in molecular, hydrogen-bonded solids (not to frequently studied today due to

intensity and resolution limitations, but a real neutron case for the future) and the *in situ* observation of metastable, nano-structured phases. However, any example is not more than an example, it is presumptuous to predict, which processes and materials will be of primordial interest in 10 years' time.

Benefits of STS

The STS will serve better longer d-spacing in diffraction (e.g. on the diffractometer VERDI) than what is available today in terms of diffractometer at FTS and HFIR. STS may provide the means to overcome the problems linked to the incoherent scattering of hydrogen, especially for solvents in liquid systems by polarization analysis. However, the approach proposed in the instrument design of EWALD would not be conceivable for this purpose at it demands very low temperatures, which is excluded due to the very nature of *in situ* experiments being conducted at real conditions.

One can expect the availability of a broad energy coverage of its spectrometers, reaching out for small Q, with an energy resolution in the range of 1%. The high $\Delta d/d$ resolution of the HighResPD instrument will be unprecedented, and of some use for chemical reactions with very subtle structural changes coming along with the chemistry. With a generally very low overall background, surely a stronghold of STS, small samples and signatures (e.g. from interfaces) will become observable, one will be able to interrogate small features. This is probably the main opportunity but not the only one of the reduced background contribution of a new state-of-art source with lower repetition rate.

Complementary Experimental Techniques

The "laboratory on the beam line" idea finds a lot of support among the community studying chemical reactions. The combination of neutron scattering, with other techniques in a simultaneous manner, is a crucial step forward beyond combining neutron diffraction and neutron spectroscopy onto a single beam line. Integrating other methods such as Roman spectroscopy and thermal methods is important, considering the difficulty of reproducing a chemical process precisely enough for separate off-line measurements.

Auxiliary Requirements

Current sample environments typically include low and high temperature, pressure and magnetic field. New capabilities can be envisioned that facilitate studies of radiation effects on samples or the application of electric fields.

For partial deuteration as well as other isotope exchange and labeling experiments corresponding laboratory facilities and expertise needs to be provided. This is a very strong feature of neutron scattering and should be used to its full extent, but the very specialized equipment and knowledge is not easily available in most academic (and commercial) laboratories.

In situ work on single crystals is easier with TOF methods then with continuous neutron sources facilitating studies in special chemical environments. Inelastic measurements of *in situ* chemical reactions at higher temperatures is desirable, but limitations of the Debye-Waller effect must be overcome.

Adapted high pressure devices should be available for all new instruments. And this is true also for other techniques of sample environment, thus, some effort in pooling sample environment rather than developing only dedicated devices is needed.

Modulated or pulsed pressure or temperature linked with stroboscopic data acquisition methods possibly provide a new way to investigate *in situ* extreme conditions and/or rapid time dependencies. In a similar way one should provide microfluidics and gas dosing linked with stroboscopy.

The experience with VISION shows what is going to come in terms of data volume of those multimodal instruments. One should prepare now for large data rate handling, and maybe profit from the number crunching experiences of laboratories such as CERN or Stanford.

Some means for an easy and streamlined data treatment should be provided. This provides an entrance door for the user community, but in the field of *in situ* experiments enables users that face enormous amounts of data (e.g., thousands of diffraction patterns). Methods are needed here to extract publishable information without too much pain in reasonable time.

3.8 ADVANCED FUNCTIONAL MATERIALS

Tyrel McQueen (chair), Johns Hopkins University; Ken Andersen, European Spallation Source; Goran Arbanas, ORNL; Dipanshu Bansal, post doc; Jonas Birk, Paul Scherrer Institute; Craig Bridges, ORNL; John Budai, ORNL; Stuart Campbell, ORNL; Bryan Chakoumakos, ORNL; Michael Crawford, DuPont Company; Michelle Dolgos, Oregon State University; Mathieu Doucet, ORNL; Panchapakesan Ganesh, ORNL; Masato Hagihara, ORNL; Raphael Hermann, ORNL; Jason Hodges, ORNL; Jiangnan Huang, student; Jiangnan Huang, student; Seth Hunter, University of Tennessee; Ashfia Huq, ORNL; Yoon Kang, ORNL; Abebe Kebede, North Carolina A&T State University; Alexander Kolesnikov, ORNL; Ivan Kravchenko, ORNL; Ana Larralde, University of Buenos Aires; Chen Li, Carnegie Institute for Science; Robin Macaluso, University of Texas, Arlington; Chrysostomos (Tommy) Michaelides, ORNL; Jennifer Niedziela, ORNL; Naresh Osti, ORNL; Ward Plummer, Louisiana State University; Abhijit Pramanick, City University of Hong Kong; Yang Ren, Argonne National Laboratory; Jeff Sakamoto, University of Michigan; Anjana Samarakoon, University of Virginia; Radha Shivaramaiah, University of California, Davis; Elinor Spencer, Virginia Tech; Shelby Stavretis, University of Tennessee; Alexander Thaler, ORNL; Shanmin Wang, ORNL; Xiaoping Wang, ORNL; Angus Wilkinson, Georgia Institute of Technology; Ziling (Ben) Xue, University of Tennessee

Advanced functional materials are complex with interesting and useful properties, with impact ranging from energy storage and designer mechanical structures, to catalysis and the discovery of new phenomena. The associated grand challenges can only be tackled with a nationwide effort that includes the use of neutrons as a unique probe of matter. The most important design criterion for new instruments at the STS is that of custom sample environment modularity: the ability to both use custom experimental setups on individual end stations, to measure materials under *in operando* conditions, and the ability to quickly and easily move the apparatuses between beam lines. The small, fragile, and reactive/toxic nature of the specimens demands specialization of individual beam lines for specific measurements, with measurements of complementary quantities accomplished by moving the experiment between end stations. Additional needs identified are that software development should be an integral part of the design process, even before beam line construction, and it is critical to provide functional laboratory space and ancillary characterization capabilities proximal to the end stations.

An advanced functional material is defined as one with an interesting and real property. They have the potential to make dreams such as individualized medicine and quantum computing a reality. In order for the promise of advanced functional materials to become a reality:

1. Methods to put every atom in its place, scalably, must be developed.
2. Functionality must be directly demonstrated (rather than inferred).
3. The connection of structure and dynamics to functionality must be made explicit.

Neutrons are uniquely suited to tackling these objectives because of their penetrating power, and ability to probe across relevant time and length scales. However, since advanced functional materials are often

highly structured, from the atomic to mesoscale, hydrogenous, absorbing, small, fragile, and reactive/toxic, the current neutron capabilities in the United States are not sufficient to meet the scientific needs.

Science Opportunities
Two areas in which neutrons are poised to make significant contributions if appropriate instrumentation and capabilities are available, are:

1. In the connecting of dynamics directly to function, particularly in catalytic cycles and transient states under *in operando* conditions;
2. In the development of thin films and devices.

Four specific instrument concepts, not currently available in the United States, are central for the STS to have impact:

1. High intensity, ultrasmall volume diffractometer/spectrometer;
2. Ultrahigh resolution diffractometer;
3. Polarized, energy-selective (0 or finite ω) single crystal diffractometer (SNS BL-12, TOPAZ/SNS BL-9, CORELLI blend); and
4. High energy resolution at low ω (short pulse/long flight path).

Benefit of the STS
The design of the STS should be based on the high level scientific and societal objectives, not on specific beam lines or techniques. In other words, the STS design should be science, not engineering, driven. Because of the small, fragile, and reactive/toxic nature of many specimens, studies on advanced functional materials will be pushing the new capabilities to their limit; the compromises inherent in building multimodal instruments will preclude them from having the impacts described above. At the same time, a holistic set of measurements across time and length scales is critical for directly connecting dynamics to function. To satisfy these apparently conflicting objectives, it is essential that beam lines and end stations be designed to allow for seamless sample environment exchangeability and modularity across the instrument suite (i.e. “Labs for Beams”). Such an approach also avoids wasted time from sample changes as experimental environments can be setup nearby prior to runs. Further, it offers the flexibility inherent in the breadth of applicability of advanced functional materials: today lasers or gas cells may be in demand. However, in the future other capabilities such as flow reactors may be necessary. It is impossible to the facility to procure and operate the wide breadth of capabilities that are needed: instead, it is essential that facility users be able to bring custom equipment on-site to carry out their studies.

Auxiliary Requirements
It is important that ensure that software is included in the design process, even before construction of individual instruments commences. Specific capabilities should include:

- Virtual beam line simulators
- Dedicated modelling and simulations
- Basic analysis tools before first users

The FTS had many issues at the beginning of user operations due to the lack of software and software capabilities. This can be avoided for the STS by incorporating software, including Monte Carlo simulations of beam line performance at an early stage where users (and future users) can explore and estimate capabilities.

In addition to design requirements specific to the STS, the working group identified two more broadly applicable criteria for any user facility (including neutrons) to have impact in advanced functional materials. The first is that it is essential to have functional laboratory space and characterization equipment proximal to instruments: measurements are only as good as the samples being measured, and without the ability to know the quality of the samples at the time of measurement, it is impossible to disentangle interesting results from sample quality issues. More generally, anything that is fragile and reactive/toxic requires careful handling, i.e. user access to well-equipped laboratory spaces as close to the instruments as possible.

The proposal review process should also be reevaluated. While the current approach of instrument-by-instrument scheduling provides convenience in scheduling beam line operations, it limits scientific impact: a mistake in instrument selection results not only in wasted beam time on that one instrument, but also a significant delay before the proper instrument can then be used. Given the rate of progress in scientific fields today, this is unacceptable. To make an impact, it is essential that scheduling be flexible and science driven: when a user shows up on-site for an experiment, they must be able to move between instruments/techniques on the fly as the science demands. This has the secondary benefit of helping with screening of samples (the sample quality issue mentioned above). While such an approach may result in less efficient use of beam time on paper, the subcommittee firmly believed that it would greatly improve scientific output in practice (as evidenced by the scientific productivity of other user facilities which have adopted this science-driven approach).

3.9 ADVANCED ENERGY MATERIALS

Angus Wilkinson (chair), Georgia Institute of Technology; Jonas Birk, Paul Scherrer Institute; Bryan Chakoumakos, ORNL; Michael Crawford, DuPont Company; Michelle Dolgos, Oregon State University; Raphael Herman, ORNL; Ashfia Huq, ORNL; Timmy Ramirez-Cuesta, ORNL; Yang Ren, Argonne National Laboratory

Scientific Opportunities

There will be an ongoing need to interrogate and understand both structure across a variety of length scales, including defects and disorder, and dynamics across a range of time scales, and how they relate to the properties of materials. With the aid of enhanced computational tools, the insights provided by neutron scattering will improve the ability to design/develop new materials with superior performance characteristics. While it is not possible to predict the specific new materials that will be of interest over the next decade, the broad classes of materials under investigation are unlikely to change on this time scale and will almost certainly include: porous solids for gas separation, purification and storage; hydrogen storage materials; materials designed for the separation and sequestration of wastes such as carbon dioxide and radionuclides; battery and fuel cell electrodes; ceramic, glass, polymer and liquid electrolytes for electrochemical energy conversion and storage applications; hard and soft magnets; catalysts for solar fuels production; catalysts for chemical production; thermoelectric materials; photovoltaic materials; optical materials including scintillators, phosphors, and nonlinear optics solids; piezoelectric and electrostrictive solids for actuator applications; structural materials for application under extreme conditions, such as nuclear fuel cladding and fusion reactor walls etc.

In situ and *in operando* characterization both of materials and catalytic processes are likely to become of increasing importance, as the examination of "frozen" chemical reactions in a catalytic process, or recovered functional materials, can easily miss features that are key to performance. The development of new sources and high performance instrumentation, providing for greater data rates, along with the supporting sample environment and infrastructure will undoubtedly better enable such studies. *In situ* neutron scattering studies are also likely to play an increasingly important role in understanding of

materials synthesis and processing, as "in beam" experiments can reveal reaction paths, kinetics, intermediates, and microstructure evolution. Once again, the development of sample environments and beam line infrastructure so that these studies can be performed in an efficient and effective fashion will be key to realizing the full potential of such approaches.

It is anticipated that "small signal" experiments will become of increasing importance. This will be driven by the need to study: a) thin films similar to those used in devices; b) interfacial structure and dynamics as this lies at the heart of heterogeneous catalysis, and is often key to device performance (i.e., the SEI layer in batteries); and c) materials that are only available in small amounts as they are prepared under extreme conditions.

Benefits of STS

Many advanced energy materials have highly complex and subtle atomic structures. For example, the phases existing close to the morphotropic phase boundaries (MPB) in many piezoelectric perovskites are very subtle distortions of the parent perovskite, and they are thought to play a key role in the high performance of compositions close to the MPB. The development of a powder diffraction capability at the STS, with a resolution similar to that offered by analyzer crystal based synchrotron instruments, will bring all of commonly stated advantages of neutrons over x-rays to bare on many complex structural problems in energy materials. The value of very high resolution is clearly illustrated by the great success of the synchrotron based instruments. This high resolution is best achieved at STS because the high brightness and low repetition rate of the source are very well matched to the long flight paths needed for world-class resolution.

An increasing emphasis on *in situ* and *in operando* studies will also be facilitated by some features of instruments at the STS. For example, the larger bandwidth, for a given path length, provided by the low repetition rate of the proposed STS is advantageous for *in situ* and *in operando* studies as all the needed data must be collected in single frame. Additionally, the longer flight paths that can be accommodated for a given band width, due to the lower repetition rate of the source, provide for more space around the instrument, which can be used to accommodate the ancillary equipment needed for complex *in situ* and *in operando* studies.

Complementary Experimental Techniques

A wide variety of complementary measurement tools should ideally be available at the beam line when *in situ* or *in operando* studies are pursued. Complementary data gathered in beam can be used to help correlate the neutron experiment with other measurements performed elsewhere or, alternatively, a complete battery of measurements performed at the beam line can avoid the sometimes highly problematic process of trying to correlate measurements made under slightly different conditions at different times and locations. Depending on the materials and processes of interest, optical probes such as Raman/infared (IR) and ultraviolet visible (UV-Vis) may be appropriate, electrical measurements such as impedance spectrometry or charge discharge curves could be of great value, the measurement of a mechanical response to an electric field may be needed, and for chemical processes gravimetric analysis, calorimetry, gas handling/mixing, and reactant analysis by mass spectrometry can all be of great value.

The development of increasingly complex sample environments and the introduction of new complementary measurement tools are likely to be demanding on both staff time and expertise. Proper attention to this issue will be essential for success as we move towards increasingly complex *in situ* and *in operando* studies.

Auxiliary Requirements

A move towards increasingly complicated sample environments, and the acquisition of complementary data in parallel with the neutron measurement, will require a high level of instrument integration and

automation. Users cannot be expected to rapidly learn the details of the hardware used for complementary measurements and then manually coordinate the successful acquisition of several different data streams.

There will undoubtedly be cases where the integration of simulation with an experiment on the fly is highly advantageous. Such simulations can be used to fine tune the experiment plan on the fly.

The high brightness of the STS along with high performance instrument designs will, in some cases, lead to a mismatch between the time needed to acquire neutron data and the time it takes for a sample to equilibrate or undergo some change. In order to make efficient use of beam time, with minimal time lost waiting on samples, instrument designs that can accommodate on the fly changes between experiments should in some cases be considered.

3.10 ENGINEERING MATERIALS

David Jacobson (chair), National Institute of Standards and Technology Center for Neutron Research; Jeffrey Bunn, ORNL; Mathew Connolly, National Institute of Standards and Technology; Kenneth Littrell, ORNL; Andrew Payzant, ORNL; Dayakar Penumadu, University of Tennessee, Knoxville; ORNL; Harley Skorpenske, ORNL; Alexandru Stoica, ORNL; Claire White, Princeton University

Scientific Opportunities

Engineering materials is a broad area that spans a range of materials and early prototype product development to understanding the lifecycle and ultimate failure modes of materials and devices in the field. The scientific and technological impact that neutron scattering can have is profound. For example, weld failures can bring down airplanes and bridges and the long term degradation of concrete will also result in catastrophic bridge collapse. Both of these areas alone account for a significant fraction of the U.S. gross domestic product. In addition neutron methods have and will continue to play a key role in stewardship of the nation's nuclear fuel infrastructure.

Advanced manufacturing has been making major innovations in product fabrication. For example, methods such as 3D printing of metal parts are revolutionizing manufacturing enabling rapid prototyping and manufacturing of new parts that are not even possible with conventional milling equipment. This method relies on building parts completely from welds. Understanding the important role of temperature during the 3D printing process is critical to develop the methods to manufacture stress free parts that will not suffer catastrophic failures. Neutron scattering can play a key role here by developing instrumentation to make rapid *in situ* measurements of stress and texture. To realize this goal it is necessary to be able to measure stress *in situ* in materials under the same manufacturing conditions with less than or equal to sub 100 μm spatial resolution and less than 100 με (microstrain) resolution. Measuring 3D strain *in situ* would further provide the critical capabilities necessary to understanding how to develop the required prescriptive manufacturing processes to create reduced strain or strain free parts. In addition to stress it is important to measure texture *in situ* as well and develop methods to separate the texture from the stress measurement. The time evolution of stress will also be important to study as parts are aged and fatigued due to use. Measurements must be made with sample environments that can vary the load, pressure and temperature. As these measurements can also take long periods of time (months-years) it is also critical to design sample environments for materials testing that can be removed and replaced on the beam line at various times for ~3 days in order to make measurements that can monitor the slow evolution of processes such as creep or the evolution of slow chemical reactions in concrete.

The length scales needed to measure new engineered materials extend from the nanoscale measurements of stressed lattices to the macroscale measurements of submillimeter structures and how they form during the manufacturing process. Studying these parts *in situ* will provide validation methods critical to finite element models developed by the materials genome initiative and other advance manufacturing initiatives

in the future. This will enable U.S. industry to maintain its competitive and innovative edge in the future world economy.

In between the two extremes of nanoscale and macroscale is the mesoscale, the most challenging scale for characterization methods to operate in. Here is where the greatest and most innovative impact characterization methods could have in materials development. Understanding precipitate formation at length scales between 50 nm and 50 μm in materials with high spatial resolution could have a significant impact on areas that have to date been largely ignored or poorly studied due to the lack of *in situ* methods. Although microscopy methods can study these length scales, these methods lack the powerful *in situ* capabilities available to neutrons to study specimens truly non-destructively. New grating phase imaging methods have recently shown promise towards measuring the spatially resolved small angle scattering distributions in materials.

Advancing the state-of-the-art measurement capabilities to allow the study of mixed mode fracture propagation by measuring the 3D distribution of stress prior to facture is of critical importance to advance understanding of fracture in materials. This area is very poorly understood due in part to the lack of *in situ* measurement technology. Neutron methods could play a key role in developing the early understanding of this process.

Understanding the lifecycle of nuclear fuel and understanding how defects affect the degradation of the fuel and other reactor components during the life of a reactor is another area that neutrons can contribute to in the future. This will be critical to understanding the safety and improving the efficiency of advanced reactors that will be critical to U.S. energy efficiency. It will be important to use neutrons to image and study nuclear fuel. Here x-ray methods fail even with synchrotron intensities. Neutron facilities are also ideal places to make measurements of spent nuclear fuel elements due to the in house expertise with radiation safety.

Understanding future advanced energy storage materials for beyond lithium-ion is important. Efficient use of natural resources and potentially better performance may be achieved using other battery chemistries based on magnesium and sodium. New *in situ* methods that can address these chemistries such as the nascent neutron phase imaging techniques could provide critical sensitivity to study these new materials and chemistries *in situ*.

The largely unexplored method of phase imaging could also provide sensitivity gains as much as 1000 to hydrogen in materials over traditional transmission base imaging methods. This could prove to be important to understanding embrittlement in materials used in pipelines and other processes where hydrogen embrittles engineering materials.

Benefits of STS

The slower pulse repetition rate each with significantly more neutrons than the first target station will allow for longer wavelengths to be used with much higher intensity that will allow for measurements of strain and texture that go beyond cubic lattices. Longer wavelengths will also allow one to measure small angle scattering and make Bragg edge strain maps.

STS complement to FTS and HFIR

As stated at the beginning, the range of problems that can be addressed with neutrons and the potential impact of discoveries is quite staggering. To fully address all of these potential impacts a very diverse neutron measurement capability is needed. A high flux continuous source like HFIR, not just pulsed sources, will be key to addressing major areas of engineering materials research. The main focus of this discussion was on the specific impact that the STS could have to dramatically extend the state-of-the-art in engineering materials. A broad range of research was discussed, but it is clear that each part or product

may bring with it a host of ancillary equipment that further complicates how one can mount and study the part with neutron scattering. With three sources at Oak Ridge it will be important to provide optimized capabilities for studying engineering materials. STS will provide long wavelengths needed for extending the range of stress and texture measurements in an instrument such as MENUS, whereas the finer resolution of the pulses from SNS will allow for the highest resolution measurements of strain in spectrometers like SNS BL-7, VULCAN. Although not currently available, a pulsed imaging facility should be built at the SNS in order to provide the United States the same access to new imaging methods such as Bragg edge imaging. Oak Ridge should also build an optimized state-of-the-art imaging facility at HIFR. Neutron imaging has played and is still playing a vital role in the development of fuel cells, batteries, concrete, geology, etc. and it was chosen as one of the lead instruments to be built at the European Spallation Source (ESS). This combination of instruments would provide an ideal suite for making measurements of engineered materials.

Auxiliary Requirements.
It is also critical to fully develop an infrastructure for 3D-real time analysis of the data. It will be critical to develop a way to fully integrate measurements with models, which is currently a difficult hurdle for users to overcome with the present state-of-the-art. Such an advancement would allow industry to better utilize the measurement capabilities at all the national laboratories. In addition, multimodal techniques like x-ray imaging and diffraction could be used *in situ* to provide complementary analysis in a new instrument.

4. INSTRUMENT AND TECHNIQUE WORKING GROUP SUMMARIES

This section contains reports from the focus groups, which centered on the future instruments at the STS. Based on the conclusions of the scientific sessions, the groups discussed instrument specifications necessary to solve the scientific challenges. The groups then discussed and ranked proposed instruments. The reports are prepared by the discussion leaders.

4.1 POWDER DIFFRACTION

Ashfia Huq (chair), ORNL; Katie Andrews, ORNL; Goran Arbanas, ORNL; Craig Bridges, ORNL; Stuart Calder, ORNL; Michelle Dolgos, Oregon State University; Antonio dos Santos, ORNL; David Freeman, ORNL; Ovidiu Garlea, ORNL; Thomas Hansen, Institut Laue-Langevin; Jason Hodges, ORNL; Camden Hubbard, Applied Diffraction Services; Seth Hunter, University of Tennessee; Richard Ibberson, ORNL; Abebe Kebede, North Carolina A&T State University; Ana Larralde, University of Buenos Aires; Kuo Li, Center for High Pressure Science and Technology Advanced Research; James Neilson, Colorado State University; Daniel Olds, ORNL; Katharine Page, ORNL; John Parise, Stony Brook University; Jeff Sakamoto, University of Michigan; Radha Shivaramaiah, University of California, Davis; Shanmin Wang, ORNL; Claire White, Princeton University; Pamela Whitfield, ORNL; Angus Wilkinson, Georgia Institute of Technology

The community of scientists in the Powder Diffraction breakout session were primarily from the solid state chemistry community most who specialize in synthesis and characterization of new functional materials with secondary interest in magnetism. A large fraction of them were faculty expected to be power users of the diffraction instruments at both HFIR and SNS and the STS. The instruments under discussion were BL-8B, RAPID, for the FTS and HighResPD and VERDI for the STS for both single crystal and powder diffraction.

RAPID is an instrument that can be located at BL-8B at the FTS. Current performance is estimated to be ~32 times higher count rate compared to POWGEN (albeit with less resolution). It is envisioned that the primary flight path of this instrument will be 35-40m with a secondary flight path of 2-2.5m. Position sensitive ^{3}He tubes will be used for detector coverage. This instrument will be ideally suited for structure refinement and total scattering of small samples, high speed parametric studies and stroboscopic studies. There was some discussion about having a Fermi chopper option similar to the NOVA diffractometer at the Japan Proton Accelerator Research Complex (J-PARC). There was a fair amount of discussion regarding the availability of various sample environments that go beyond simple temperature control and that these should be integrated within the design criteria of the instrument. Given the fast data acquisition expected, new sample environment concepts will be required to reduce the time spent controlling things like temperature, pressure, gas flow, etc. to maximize the use of beam time. It was discussed that currently on SNS BL-1B, NOMAD, and SNS BL-11A, POWGEN, often temperature changes take significantly longer time than the measurement itself and so addressing this is critical. It should be easy to switch out sample environment and the instrument design should also take that into consideration.

HighResPD is a high resolution powder diffractometer proposed for STS. Given the lack of such an instrument in the United States, that gives synchrotron like resolution, it was deemed a very high priority instrument for this community. It is widely accepted that the structural questions that are being solved from these new diffraction instruments are getting more and more complex and as a result the need for high resolution is greater than ever before. This instrument is expected to have a primary flight path of 100-120m to gain the high resolution of $\Delta d/d = 0.035\%$. Rietveld refinement of a typical sample of ~0.5g is expected to take ~1hr collection time.

The concept of VERDI was discussed in detail. This is an instrument concept that allows measurement of both powder and single crystal primarily targeted to magnetic materials. The user base will consist of condensed matter physics community studying correlated electron phenomenon. The sample environment requirements for this instrument will be a field of 14T, with 10GPa pressure and mK temperature. This instrument concept also calls for a monochromatic mode supported by a Fermi chopper to improve signal-to-noise as needed for small moment measurements. Further evaluation is needed to answer if polarization options should be built in or movable.

Overall data needs for these instruments were also discussed. It is clear; data treatment of polarized data would have to be worked out for VERDI. Live data viewing and analysis is clearly at the top of the requirements without which these high throughput and high speed instruments would not be used effectively. It was also discussed that all data stream should be tied together to correlate sample environment variables seamlessly with the diffraction data. Overall, the consensus for prioritization was that the highest priority instruments were RAPID and HighResPD with second priority being VERDI.

4.2 SINGLE-CRYSTAL DIFFRACTION

Bryan Chakoumakos (chair), ORNL; Annette Bodenheimer, North Carolina State University; John Budai, ORNL; Claudia Cantoni, ORNL; Huibo Cao, ORNL; Julian Chen, Los Alamos National Laboratory; Leighton Coates, ORNL; Matthew Cuneo, ORNL; Lawrence Falvello, University of Zaragoza; Oksana Gerlits, ORNL; Masato Hagihara, ORNL; Zhen Huang, Georgia State University; Choel Kim, Baylor College of Medicine; Andrey Kovalevsky, ORNL; Yaohua Liu, ORNL; Robin Macaluso, University of Texas, Arlington; Flora Meilleur, ORNL/North Carolina State University; Brad O'Dell, North Carolina State University/ORNL; Abhijit Pramanick, City University of Hong Kong; Marc Pusey, iXpressGenes, Inc.; Don Ronning, University of Toledo; Stephan Rosenkranz, Argonne National Laboratory; Richard Sayre, Los Alamos National Laboratory; Elinor Spencer, Virginia Tech; Alexander Thaler, ORNL; Wei Tian, ORNL; Venu Vandavasi, ORNL; Xiaoping Wang, ORNL; Kevin Weiss, ORNL; Christoph Wildgruber, ORNL; Ming Yi, University of California, Berkeley

The community of scientists in the Single-Crystal Diffraction breakout session was evenly divided between two communities with interests in either macromolecular structures ("large unit cell") or small unit cell structures. The small unit cell community was particularly interested in extreme conditions and magnetic structural studies. The large unit cell community was particularly interested in high-resolution structural studies of macromolecular crystals, and the utilization of "sample environment" to polarize the hydrogen-atoms in the samples and thereby dramatically improve the signal-to-noise and sensitivity to the hydrogen-atoms. The breakout began with a brief overview of the ORNL three source strategy and the specifications for STS together with the implications for single-crystal diffraction and the current single-crystal diffraction instrument suite. The instruments under consideration for this breakout session were primarily EWALD, VERDI, and NeSCry. Dynamically polarized crystallography (DyPOL) is an essential option for EWALD to dynamically polarize the hydrogen nuclei in the samples. NeSCry and VERDI are similar for single-crystal studies, but because VERDI would also accommodate powdered samples, VERDI was a clear favorite from the community interests.

EWALD. The science case for neutron macromolecular crystallography is based on the premise that a fully optimized instrument will open new frontiers in structural biology by enabling x-ray sized crystals (of ~100 microns or less major axis) to be studied. Given that the protonation states and hydrogen-bonding interactions of proteins are key to understanding structure and function mechanisms. Neutron diffraction can play a vital role in determining accurate hydrogen positions in macromolecules. However, the large unit cell size and small crystals that are typical of most macromolecular systems gives rise to generally weak diffraction and poor signal-to-noise that is effectively drowned out by the large incoherent background form the hydrogen atoms. Hence, there have been multiple challenges: to fully deuterate protein crystals, grow large sized crystals, and build neutron diffractometers on more powerful neutron sources. The thermal neutron cross-sections of hydrogen depend strongly on the degree of nuclear polarization has been known for long time and the benefit of controlling polarization in hydrogenous samples has been demonstrated more than once (perhaps the first one being that of Hayter et al. 1974 *Physical Review Letters* **33**, 696). For a crystal with polarized hydrogen nuclei studied with a polarized neutron beam, the hydrogen incoherent contribution is reduced to zero while the hydrogen coherent cross-section is simultaneously enhanced 8-fold. This effectively removes the limitations of sample background limited diffraction, while simultaneously amplifying the hydrogen coherent contribution to the diffraction data. This so-called dynamic nuclear polarization of the sample as an option DyPol on a single-crystal diffractometer such as EWALD on the STS would create a game-changing instrument capable of opening a new frontier in neutron structural biology. Current neutron crystallographic studies of macromolecular crystals typical take several days to several weeks when even feasible, whereas EWALD with the DyPol option could produce a complete dataset in one day. EWALD would view a high-peak-brightness moderator at a distance of ~90 m using a polarized beam with a wavelength range of ~4.3 A, and have a large coverage of Anger cameras (<0.5 mm resolution and robust to magnetic fields). The raw flux of EWALD on the STS would be 75 × that of MaNDi on the FTS. A prototype DyPol is being developed now at ORNL through laboratory directed reserved and development (LDRD) funding, and this will be tested on HFIR CG-4D, IMAGINE, by the end of the fiscal year. Given the ongoing developments in the components needed to make a compact and efficient DyPol a reality, and strong collaboration with experts at the National High Magnetic Field Laboratory (NHMFL), the community support to push this instrument concept forward is stronger than ever. The STS can make this 40 year-old instrument concept a reality.

VERDI is a long-wavelength neutron diffractometer for primarily magnetic structure determination similar to the ISIS-TS2 WISH instrument, but with a 5-fold increase in flux. VERDI would be optimized to study magnetic structures with high-resolution at low-Q for both single-crystal and powder samples under extreme conditions of temperature (mK – 1000K), pressure (diamond-anvil cells), or magnetic field (14 T). Polarization of the incident beam (dedicated or optional) with optional polarization analysis of

diffracted beams would be an essential feature of the instrument. VERDI would be situated on a high-peak-brightness coupled moderator, and utilize 0.5 mm spatial resolution detectors that are robust to magnetic fields. VERDI's game changing capabilities are the ability to study small crystals, on the order of 0.1 x 0.1 x 0.1 mm^3, with combined extreme conditions: mK – high magnetic field, high pressure – low T, high T – high magnetic field.

The working group's clear priority list was that both EWALD (with DyPol option) and VERDI should be built. Ultimately, the community selected the instruments with perceived game-changing scientific capabilities. EWALD with DyPol option will greatly improve the signal-to-noise (>100-fold) of the diffracted beams and, thus, enable high-resolution crystallography on unprecedentedly small, and fully hydrogenous crystals. VERDI will greatly expand extreme environment (high pressure, high magnetic field, ultra-low temperature) single-crystal and powder studies with optional polarization analysis.

4.3 SANS

Volker Urban (chair), ORNL; Robert Briber, University of Maryland; David Cowburn, Albert Einstein College of Medicine; Mark Dadmun, University of Tennessee; Lisa DeBeer-Schmitt, ORNL; Changwoo Do, ORNL; Morten Eskildsen, University of Notre Dame; Millicent Firestone, Los Alamos National Laboratory; Yun Han; William Heller, ORNL; Joanna Krueger, University of North Carolina, Charlotte; Susan Krueger, National Institute of Standards and Technology; Ken Littrell, ORNL; Ryan Oliver, ORNL; Bradley Olsen, Massachusetts Institute of Technology; David Worcester, National Institute of Standards and Technology Center for Neutron Research/University of Missouri

The session strongly endorsed the NScD three-source strategy. Within that context attendees concluded that the cold source at HFIR will remain the best place for "classical" SANS applications, in particular those that push to the smallest achievable scattering vectors. Therefore, the three-source strategy must have a strong focus on optimizing SANS instruments at HFIR and pushing them to the game-changing next level. The session participants discussed two instrument concepts at HFIR that pursue this goal, being complementary to each other and to current and future SANS capabilities at the FTS and STS. These two concepts were for the purpose of the breakout discussion termed "VSANS" and "SBSANS" and are similar in their specifications to the BARNS and FLOODS concepts, respectively, which have been developed previously by NScD.

In addition, the breakout session participants determined a clear case for additional SANS instrumentation at the STS. The SWANS concept is the best aligned instrument concept because it is uniquely possible at the STS and, therefore, provides capabilities that will be complementary to the upgraded HFIR SANS instrument concepts. The session emphasized that it must be ensured that a SWANS instrument will serve all of the scientific communities, including quantum condensed matter, metallurgy, soft matter and biology. This is of particular importance if only one such instrument is initially constructed at the STS. This instrument would go a long way to reduce the queue of users for medium sensitivity SANS.

The SANS instruments discussed by the session attendees cover a wide range of science themes, including hard condensed matter, mineralogy, geology, soft matter, and biology. In more detail the session recommended that VSANS would provide needed capabilities for hard condensed matter, mineralogy, geology, and those soft matter applications that are not well suited for SBSANS. On the other hand the complementary specifications of SBSANS would be optimized for biology and a large fraction of soft matter research.

The breakout discussion gave top priority for pushing the SANS capabilities at HFIR. Among the two concepts discussed for HFIR (VSANS/SBSANS or BARNS/FLOODS) no ranking was applied, because both instruments would serve different, important science communities. For the STS, the SWANS

concept was ranked first under the assumption of a three-source strategy. Without the optimization of HFIR SANS instruments as part of the three-source strategy, the outcome would be radically different; for example requiring much more attention to the development of low-Q optimization at the STS SANS.

Key Parameters

VSANS at HFIR (parameters similar to BARNS)

- Adaptable sample area gap: 0 – 1m (soft: rheometer) 2m (for polarization for background reduction), adjustable table height, tilt, rotation
- Sample size: 1cm x 0.1-1mm thick
- Beam size (for scanning ability): 1x1mm down to 0.1x0.1mm^2
- Q-range: 0.0001 – 1.0 Å^{-1}; $Q_{max}/Q_{min} > 500$ (single shot)
- Q-resolution: dQ/Q: 10% or less
- Wavelength range: cold source, 20A
- Polarization and analysis

SBSANS at HFIR (parameters similar to FLOODS but focus on sample is an OPTION, not fixed)

- Adaptable sample area gap: 0 – 1m (soft: rheometer) 2m (for polarization for background reduction), adjustable table height
- Sample size: **30 microliter or less (game changer, similar to SAXS);** 1mg/ml, [low-intensity scattering sample], ~0.01cm^{-1} must be measurable in hrs. signal "observable" in 15-30 minutes in D_2O. **Changeable optional optics for focus on sample**.
- Time-resolved <1 min for 1cm^{-1} intensity
- Q-range (single shot): 0.001 – 0.4; (Q_{min}~0.005 for FLOODS option ok)
- Q-resolution: dQ/Q: 10-15%
- Low intrinsic instrument background; (polarization-analysis to remove incoherent background)
- Wavelength range: whichever works best (highest flux, but also consider wavelength-dependence of inelastic scattering)

SWANS at STS

Key parameters are essentially those of the HiRes-SWANS concept developed previously. The breakout session emphasized that SWANS at STS must provide

- A sample area that provides flexibility for sample environments that serves all science communities including quantum condensed matter, metallurgy, soft matter and biology.
- Include the capabilities of a low-Q Diffractometer that serves the membrane science community among others. The required instrument specifications for this purpose appear to be a subset of what SWANS will be able to provide and they include the following:
  - Sample size: 1 – 100 ul
  - Q-range (single shot) 0.01-6/A
  - Q-resolution: dQ/Q: SWANS 1%

Sample Environment

VSANS at HFIR (similar to BARNS)

- T: 50mK – 1200K
- Magnetic Field: 10T
- Pressure: for magnetism (flux lattices) 10GPa; for geology: uniaxial 10MPa compression with 50MPa isotropic
- Synchronous *in situ*/in-beam techniques: stress/strain, electric resistivity, AC susceptibility, heat capacity etc.

SBSANS at HFIR (similar to FLOODS)

- User supplied sample environment needs to be plug-play into data acquisition and utilities (standard mounting)
- T: 4C – 100C standard, -80C freezer (pharma), liquid nitrogen
- Synchronous techniques Fourier Transform-Infrared, optical spectroscopy, circular dichroism, UV-vis – for kinetic/time-dependent studies
- Humidity control
- *In situ* chromatography
- Magnetic field: not much used, low fields (permanent magnet), zero-field could be interesting
- E-field: gel-electrophoresis
- Pressure: Ocean vents biology, p-induced protein folding 2-10 kbar

Flexibility for sample environments that serves all science communities including quantum condensed matter, metallurgy, soft matter and biology (see combination of requirements specified for VSANS and SBSANS above). In the longer term, flow mixing cells may be usable, as the sensitivity increases. Outside the specific environment issue, high quality and rapid data analysis, reduction, and simulation can improve throughput and provide better scientific focus.

Top Instruments

The breakout participants' discussion went beyond considering complementing existing instruments and made clear recommendations for upgrading existing HFIR instruments in addition to recommending building SWANS at the STS. All three instrument concepts complement each other with regard to capabilities. Somewhat simplified, they map onto the suite of instruments laid out in a previous report[1]: BARNS, FLOODS, SWANS. VSANS (BARNS) will have the lowest available scattering vector, SBSANS (FLOODS) will have a more standard continuous wave SANS Q-range with an emphasis on high flux and low background and optional focusing capability at the sample for small sample volumes of low-intensity scattering samples, and SWANS will have the highest dynamic Q-range and the sharpest Q-resolution (dQ/Q), particularly in its higher Q-range.

4.4 REFLECTOMETRY

Gregory Smith (chair), ORNL; Haile Ambaye, ORNL; John Ankner, ORNL; Mathieu Doucet, ORNL; Michael Fitzsimmons, ORNL; Panchapakesan Ganesh, ORNL; Tonya Kuhl, University of California, Davis; Rajeev Kumar, ORNL; Hans Jochen, Lauter; Valeria Lauter, ORNL; Chris Leighton, University of Minnesota; Liyuan Liang, ORNL; Brad Lokitz, ORNL; Jaroslaw Majewski, Los Alamos National Laboratory; Steve May, Drexel University; Roger, Pynn, Indiana University; Xi Tong, ORNL; Bogdan Vacaliuc, ORNL; David, Worcester, National Institute for Standards and Technology Center for Neutron Research

The breakout session began with a brief discussion of the proposed STS target and coupled hydrogen moderator design and the resulting source parameters for long wavelength neutron studies. Then, based on the calculated source performance plus new instrument designs, four instrument concepts were presented as a basis for discussion of reflectometer concepts to meet the needs of the scientific community.

The first instrument discussed was a high speed kinetics reflectometer design called the Quicker Reflectometer (QIKR). This instrument is proposed to study time-resolved processes of thin films and interfaces. This instrument concept is based on a short source-to-sample distance which, when combined with the low repetition rate of the STS source, produces a wide usable bandwidth. The large bandwidth permits measurements of the reflectivity over a large Q range for each pulse of protons on target. This makes QIKR ideal for studies of kinetics and time dependent processes such as self-assembly of

surfactants, polymers, and proteins at solid and liquid interfaces; rearrangement processes in thin films such as polymer interdiffusion, inter-layer movement, lipid flip-flop, and annealing/drying/exchange/wetting processes in composite films such as those used in photovoltaic applications; and encapsulation and release of components in plastics, polymer blends, drug delivery and implant materials to name a few.

Based on sample measurement time, the overall gain in performance for QIKR is estimated to be as high as 100X SNS BL-4B, Liquids Reflectometer. QIKR addresses needs for kinetics at surfaces and interfaces and as presented is a very simple instrument with simple optics providing the beam form the source. The group was very enthusiastic for the QIKR instrument as presented. They also suggested that additional gains may be obtained by including up-stream focusing optics (e.g. mini-SELENE or parabolic optics).

Another two instrument concepts were presented and discussed which are optimized for delivering a focused bright beam at the sample position. Both of these concepts are aimed at studies of small samples and/or small sample features. The first concept is the Magnetism Second Target Advanced Reflectometer (MSTAR). On MSTAR, the beam is delivered to the sample by a vertically converging, set of elliptical neutron mirrors. The elliptical shape is approximated by flat supermirror sections of varying reflectivities (from m=4-6). Horizontally, the optics consists of straight or curved guide sections. This delivers a beam at the sample position with a high divergence in the out-of-plane direction and "normal" divergence in-plane. For specular reflectivity, all of the high divergence can be used thus increasing the total flux at the sample. At the same time, the beam may be polarized in the in-plane direction by an insertable flat polarizing optic.

Another design concept discussed for focused beams on small samples was the Variable Profile Beam Reflectometer (VPBR). The basic idea is similar to MSTAR. The major difference in the suggested focusing optics would be based on the SELENE design proposed for the ESTIA instrument at the ESS. In this design, the neutrons are point-to-point focused both vertically and horizontally by a double set of elliptical mirrors in each plane. The divergence at the sample position is controlled by sets of apertures in the guide system. For both MSTAR and VPBR, the source to sample distance would be much larger than for the QIKR instrument because of the distance needed to accommodate the novel optics so frame definition choppers would be employed to increase the wavelength bandwidth as needed. For both concepts, for small samples, the gains achieved with the optics on a small sample could be as much as much as 200X the SNS BL-4A, Magnetism Reflectometer.

Scientific problems which could be studied with MSTAR and VPBR include: new generation heterostructures formed by integrating topological insulators (TIs) with conventional materials; nature of the exchange coupling in multifunctional oxide heterostructures such as magnetoelectric multiferroic, BiFeO3, exchange coupled to a ferromagnet; kinetics and relaxation of domains and remagnetization in nanostructures and multilayers; non-linear rheology in cone-and-plate geometry; and combinatorial surfaces structures imposed by nanopatterned surfaces.

The fourth instrument concept discussed was the Wide and Small Angle with Big Intensity Instrument (WASABI). The WASABI design addresses needs for exploring surface features using grazing incidence small angle scattering (GISANS) and grazing incidence diffraction (GID). The design concept provides high-resolution 3D magnetic and non-magnetic structural determination with depth sensitivity and access to a lateral scale over ranges from nano- up to sub-millimeters. These techniques are important for resolving in-plane nanoscale structures at surfaces and interfaces. Similar to QIKR and MSTAR, WASABI has a focusing optics system upstream of the sample. However, in the case of the WASABI concept, the combination of elliptical and "lobster-eye" optics focus the beam in the sample plane with the focus at the detector position. Thus, the in-plane optics is similar to SANS optics. Out of plane, the

optics would be straight or curved guides to define the angle of reflection on the sample. A ^{3}He polarizer will provide the option for delivering spin-polarized neutrons to the sample. With these optics, one may simultaneously measure the specular reflectivity, the off-specular reflectivity, and the in-plane scattering which may resolve the 3D structure in thin films and interfaces. The gain for measuring the off-specular and GID components could be as high as 200X the Magnetism Reflectometer.

The types of experiments enabled by the WASABI concept would include functional oxide materials with exceptionally high ionic transport; in-plane structure in biomembranes such as lipid rafts; topologically protected spin textures in memory technologies for development of novel materials that can mediate skyrmions; exchange-coupled composite elements comprising soft and hard layers; rheology studies of liquids and soft matter; origin of flexomagnetism; self-assembly of colloids at charged surfaces; influence of charged surfaces on magnetic phase separation in films; influence of ion implantation (which is non-uniform with depth) on phase separation in oxygen dispersion strengthened steel and on stabilization of skyrmions; and the response of confined ferrofluids to magnetic fields. During the discussion of this concept, the discussion group recognized that there is potential for overlap with GISANS instruments proposed in the SANS breakout session.

For any of the four instrument concepts, it was recognized that there are several key requirements common to each which will ensure the success of such a reflectometer. They include: (1) variable spaces for insertion of optical devices; (2) flexibility at the sample position with an optical bench design; (3) deflection mirror for liquid/liquid interfaces; (4) ability to switch from polarized to unpolarized configurations; (5) capability for horizontal geometry; (6) 2D detectors for off-specular scattering (e.g. ^{3}He 2-dimensional position-sensitive detector with 1mm spatial resolution and 20 cm X 20 cm size capable of 5–10 M counts/s peak); (7) a dedicated wet lab for each instrument; (8) dedicated support for sample environment; and (9) SE technique experts included instrument design team.

Other recommendations made by the breakout group were to explore advanced background discrimination (e.g. with a correlation chopper) and other moderator designs. In addition to the cold coupled moderators, a composite moderator might perform better for VPBR and a very cold neutron (VCN) moderator for M-STAR/VPBR and WASABI.

Sample Environment

The session attendees agreed that a key part of producing the best science with a reflectometer is the availability of advanced sample environments. It was recommended that any reflectometer built will be designed with common sample position parameters so that the same sample environments may be used on every instrument. Some of the environments discussed were:

1. Solid/liquid cells
2. Electrochemical cells
3. Temperature 1.5K- 1250K
4. Mag fields +/- 5T both vertical and horizontal (up to 30 T as available)
5. Pressure 200Mpa at 200C; up to 2GPa
6. Ultra-high vacuum system with gas handling capabilities
7. Rheometer
8. Flow shear cell
9. Light illumination
10. Electric fields to 1 kV
11. Langmuir trough

Combined with these environments, the capabilities to make time-resolved measurements will not only enable diffusion or chemical kinetics experiments but also pump-probe experiments.

These concepts will meet the needs of several current and future scientific communities. They address scientific problems in biology and biomembranes including protein/membranes structure/interactions; response of polymer membranes and thin films to static and time-dependent applied fields including shear, chemical potential, and electrical fields; self-assembly of surfactants and biomimetic materials; magnetism and magnetic thin film; topological insulators and magnetic heterostructures; development of interfacial magnetism; and more.

After the discussions on capabilities and performance, it was agreed that the STS will provide neutrons with beam characteristics extremely well matched to a neutron reflectometer. So, all three concepts were highly recommended. However, since the charge to the working group was to rank the instruments, the QIKR instrument concept was ranked first. The simplicity of the instrument combined with the estimated gains and the widest unchopped wavelength band made it very attractive as the initial workhorse instrument.

Key Instruments

It was agreed that if built, the planned instruments will far exceed the FTS reflectometers' performances plus add new measurement capabilities, so it will be important to consider multiple instruments at the STS early in the project. The ideas and science covered in the MSTAR, VPBR, and WASABI instruments are very attractive. Since the VPBR and MSTAR instruments have similar concepts using focused beams to produce small variable spot sizes, it was recommended that the two concepts be combined and further studied for optimization. The WASABI instrument also covers new science using grazing incident techniques. Therefore, it was recommended that one grazing incidence instrument and one small spot size be strongly considered as the number two ranked instruments from this breakout session.

Summary

- Four instrument concepts QIKR, VPBR, MSTAR, and WASABI were presented and discussed. Two of the concepts were similar so it was recommended to perform further calculations to compare the merits of each.

- The final ranking of the instrument included three instrument types:
  - Kinetics at surfaces and interfaces (QIKR) (Ranked number 1)
  - Small Samples (MSTAR and VPBR) (Tied for number 2)
  - GI-SANS and GID (WASABI) (Tied for number 2)

- It will be important to consider multiple reflectometers in the early development of the STS. It is expected that STS reflectometers will well outperform the FTS reflectometers and likely replace them.

- The three types of reflectometers discussed will open up new scientific possibilities for the studies of surfaces and interfaces for materials science, hard condensed matter, soft matter and biology at the mesoscale.

4.5 DIRECT GEOMETRY SPECTROMETERS

Mark Lumsden (chair), ORNL; Douglas Abernathy, ORNL; Adam Aczel, ORNL; Dipanshu Bansal, post doc; Chris Chapman, Georgia Institute of Technology; Songxue Chi, ORNL; Andrew, Christianson, ORNL; Lowell Crow, ORNL; Pengcheng Dai, Rice University; Georg Ehlers, ORNL; Jaime Fernandez-Baca, ORNL; Bruce Gaulin, McMaster University; Chad Gillis, ORNL; Garrett Granroth, ORNL; Sara Haravifard, Duke University; Raphael Hermann, ORNL; Tao Hong, ORNL; Marc Janoschek, Los Alamos National Laboratory; Young-June Kim, University of Toronto; Alexander Kolesnikov, ORNL; Jonathan Leiner, ORNL; Chen Li, Carnegie Institute for Science; Masaaki Matsuda, ORNL; Rob McQueeney, Iowa State University; Adam Moule, University of California, Davis; Martin Mourigal, Georgia Institute of Technology; Stephen Nagler, ORNL; Jennifer Niedziela, ORNL; Raymond Osborn, Argonne National Laboratory; Andrei Savici, ORNL; Matthew Stone, ORNL; John Tranquada, Brookhaven National Laboratory; Jinchen Wang, University of Kentucky; Meng Wang, University of California, Berkeley; Travis Williams, ORNL; Barry Winn, ORNL; Igor Zaliznyak, Brookhaven National Laboratory

The community of scientists in the Direct Geometry Spectrometers breakout session were primarily from the condensed matter physics community most of whom specialize in the use of INS in the study of lattice and magnetic dynamics. Two staff from the NHMFL who provided valuable information about possible magnet technologies for the ZEEMANS instrument attended the session. The breakout began with a brief overview of the ORNL three-source strategy and the specifications for STS together with the implications for Direct Geometry Spectrometers and the overall INS suite of instruments. The instruments under consideration for this breakout session where primarily CHESS, HERTZ, and ZEEMANS although there was also discussion of the XTREME-X instrument as well.

Despite the fact that XTREME-X is an indirect geometry spectrometer, the scientific case for this instrument revolves around the use of complex sample environment such as magnets and pressure cells. As such, the scientific community of interest for XTREME-X overlaps strongly with the attendees present in the breakout session. The discussion centered on whether the XTREME-X concept would be better implemented by the proposed MANTA triple-axis spectrometer for HFIR. Both instrument concepts employ a CAMEA-like secondary spectrometer with multiple channels of analyzers scattering vertically and multiple final energies within a channel. This provides wide angular coverage within a plane together with a number of final energies measured simultaneously. XTREME-X, as an indirect geometry spectrometer employs TOF with the broad bandwidth provided by STS while MANTA uses a high flux monochromatic incident beam. The conclusion of the working group was there appears to be advantages of both instrument concepts and the relative performance of the two instruments cannot be compared without more detailed instrument simulations. One specific concern raised about the XTREME-X concept is that large, complex sample environments combined with a broad bandwidth incident beam could result in considerable background and, perhaps, a large number of spurious scattering events.

CHESS employs focusing optics to enable measurements with medium energy resolution on small samples (cross-sectional area of $1mm^2 - 1cm^2$). As such, it allows measurements on materials where only small crystals can be obtained or those where sample size is limited due to sample environment constraints, for instance, pressure cells. Current performance estimates yield overall gain factors of ~200 when compared to the current SNS BL-5, CNCS. It is important to note that the performance gains come at the expense of relaxed wave vector resolution. The current concept also allows for the possibility of polarized measurements. Scientifically, the breakout participants were excited about these gain factors and the potential for performing experiments on samples of this size. It was noted that the condensed matter physics community is a sample-driven community: samples are typically small shortly after their discovery and, sometimes, it is technically impossible to grow larger crystals. CHESS will open up a

broad range of scientific opportunities as there are areas where INS is, currently, just not possible due to sample size requirements.

HERTZ is a direct geometry spectrometer designed to deliver a large, homogeneous incident beam of dimensions 5x5 cm^2 with good energy and wave-vector resolution. This instrument will have advantages in problems where careful dispersion measurements or lifetime measurements are important such as in energy related materials. There was general consensus in the breakout session that the beam size as specified was too large and a cross-sectional size of 1 square inch would be sufficient. HERTZ, much like CHESS is designed to enable polarization analysis and there was an interesting discussion regarding the possibility of polarizing the instrument permanently. It was argued that there may only be a factor of two flux difference and that the polarized optics could be better optimized giving potentially much larger performance gains for polarized measurements. The consensus, however, is that there would be little gain in polarization efficiency over a design where the incident beam polarizer was driven in by motor control as is commonly performed on a triple-axis spectrometer. In addition, it was mentioned that both HERTZ and CHESS would most likely be vacuum tank instruments, unlike SNS BL-5, CNCS and SNS BL-14B, HYSPEC, as the gain in instrument background outweighs the complications of sample changes in a vacuum tank. In either case, scattered beam collimation will likely be in the form of 3d printed collimators as currently underway for SNS BL-16B, VISION.

Finally, ZEEMANS is a multimodal beam line integrated around a high field magnet. This magnet should be designed to operate in fields from 35-40 T. The possibility of an all superconducting magnet using recently developed high-T_c conductors is quite appealing as it reduces the cost (particularly the operating/infrastructure cost) significantly. Colleagues from NHMFL in attendance discussed the high-T_c option including some of the parameters that will need to be optimized and encouraged the group to define the specifications as soon as possible. It was noted that at the Helmholtz Zentrum Berlin workshop to discuss scientific opportunities for their 25 T magnet many of the science examples presented actually needed fields in excess of 30 T suggesting that ZEEMANS is in an ideal field range for a large number of scientific problems. The magnet geometry was also discussed with one suggestion to stay with a horizontal field magnet (as opposed to a split coil) as it allows the highest fields. Possibilities with pulsed magnets were also discussed but it was concluded that INS in pulsed magnets was not feasible. The combination of an array of neutron scattering techniques together with a magnet in the 35-40 T range would be truly unique scientifically. One specification note: the minimum incident energy is currently listed as 10 meV and it should clearly be less – most likely in the CHESS/HERTZ range.

There was some extensive discussion of polarized neutron capabilities related to these instruments. It was mentioned that half polarized measurements can provide useful information in a number of scientific problems. Polarizing optics would definitely be preferred over ^{3}He technology for polarizing the incident beam. As for overall optimization of the polarized neutron suite, it was suggested that Larmor techniques would provide an ideal complement to the direct geometry spectrometers. These techniques, however, are best implemented at HFIR.

As no clear priorities emerged from the discussion, a vote was held to determine a priority list. There were votes for all three instruments, indicating the importance of all instrument concepts to the community. However, the selected priority was CHESS with ZEEMANS slightly behind and HERTZ in third place. Ultimately, the community selected the instruments with perceived game-changing scientific capabilities; for CHESS enabling INS on samples of smaller size than can currently be achieved and for ZEEMANS, the ability to perform inelastic scattering, diffraction, and SANS in fields up to 40 T.

4.6 HIGH-RESOLUTION BACKSCATTERING AND NEUTRON SPIN ECHO

Eugene Mamontov (chair), ORNL; Shiwang Cheng, ORNL; Malcolm Cochran, Juelich; Antonio Faraone, ORNL; Richard Goyette, ORNL; Sudipta Gupta, University of Tennessee, Knoxville; Kenneth Herwig, ORNL; Kunlun Hong, ORNL; Ilia Ivanov, ORNL; Yoon Kang, ORNL; Maciej Kawecki, Uppsala University; Ivan Kravchenko, ORNL; Jyotsana Lal, Louisiana State University (LaCNS); Seunghun Lee, University of Virginia; Yun Liu, National Institute of Standards and Technlogy/University of Delaware; Chrysostomos (Tommy) Michaelides, ORNL; Naresh Osti, ORNL; Ward Plummer, Louisiana State University; Dieter Richter, Juelich; Lee Robertson, ORNL; Anjana Samarakoon, University of Virginia; Gerald Schneider, Louisiana State University; Shelby Stavretis, University of Tennessee; Ziling (Ben) Xue, University of Tennessee; Panchao Yin, ORNL; Yang Zhang, University of Illinois, Urbana-Champaign; Jinkui Zhao, ORNL; Piotr Zolnierczuk, Juelich

Four instrument concepts were discussed during this breakout session: a high-resolution NSE, a wide-angle NSE, a high-resolution mica-based backscattering spectrometer, and a very wide-dynamic range spectrometer with micro-eV resolution at the elastic line.

It was pointed out that NSE instrumentation priorities were discussed at a recent (May 2015) NSE workshop held by NScD. The conclusion, shared by all the session participants, was that a high-resolution (IN15-type) spectrometer would be a priority for HFIR, as a part of the three-source strategy. A prerequisite for a successful spectrometer of this type at HFIR would be a high-flux of long-wavelength neutrons from the source. Slow dynamics in complex biological and soft matter systems is the main science driver for such a spectrometer. Routine data collection at Fourier times of several hundred nanoseconds, with a possibility to reach Fourier times beyond a microsecond would be desirable, and provide unparalleled access to time scales of motion otherwise unavailable. It was noted that critically important expansion of the NSE user community would require significant shortening of the typical experiment duration from the current average of 10-14 days at the existing NSE spectrometers.

A wide-angle NSE option was discussed briefly. Such a spectrometer would address a critical deficiency of the existing NSE spectrometers that tend to measure signal at one Q value at a time. The existing spectrometer of this kind, IN11 at Institut Laue-Langevin (ILL), is advertised as capable of achieving 4 ns Fourier time, but only 2 ns is typically practical. The consensus was that further discussion of this NSE option should be postponed until 2-3 years from now, when a new WASP spectrometer at ILL will be commissioned and tested. If it demonstrates a successful proof-of-principle, reaching near 50 ns Fourier time as advertised, then a possibility of building such a spectrometer at the STS deserves further consideration.

Given that a high-resolution NSE spectrometer should be considered for HFIR, the main discussion of the first day high-resolution options for the SNS STS revolved around a high-resolution mica-based backscattering spectrometer (MBARS) and a very wide dynamic range spectrometer with micro-eV resolution at the elastic line (BWAVES). Both of these spectrometers utilize a novel wide-angle velocity selector device, WAVES.

MBARS is designed to feature a 200 neV energy resolution while maintaining a reasonably wide dynamic range of plus-minus 0.050 meV. This is achieved by employing mica analyzer crystals in near-backscattering geometry. A long wavelength at the elastic line (20 Angstrom) poises challenges to minimize the amount of structural materials (e.g., guide aluminum windows) in the incident beam, yet provides opportunities to reduce the minimum accessible scattering momentum transfer by a factor of 3 compared to the existing silicon-based backscattering spectrometers (from 0.20 to 0.06 inverse Angstrom). Such a possibility, along with the energy resolution at the elastic line beating the best existing reactor-based backscattering spectrometers by a factor of 3-4, was enthusiastically supported by the

colloidal science research community, which at present has to rely on the relatively inefficient NSE measurements at Q below 1 inverse Angstrom for their research. It was pointed out that MBARS would be much appreciated by the user base of the existing backscattering spectrometer at the FTS, if it improves the energy resolution by a factor of 15, while preserving the useful dynamic range within a factor of 2. Besides the improved dynamic characteristics, the other highly sought after option is a reduction of the beam size on the sample. It was pointed out repeatedly that the present standard sample size of 3 cm by 3 cm effectively precludes experiments on many systems (primarily biological) that cannot be obtained in sufficient quantities. The target for MBARS is to have a sample size between 0.5 cm by 0.5 cm (optimal) and 1 cm by 1 cm. Such a small sample size is also better compatible with extreme sample environments such as very high pressure cells.

BWAVES is designed to have the same small beam size and the angular detector coverage identical to those of MBARS. The energy resolution of BWAVES is about 0.003 meV at the elastic line, while its maximum energy transfer extends beyond 500 meV, limited only by the precision of the T0 chopper operation. Importantly, 5 orders of magnitude coverage of energy transfers is achieved in a single spectrum. Together with MBARS, BWAVES will yield spectra covering 6-7 orders of magnitude of energy transfers, providing seamless signal overlap at all Q values due to the identical angular detector coverage. Because of the identical beam size, it is envisioned that BWAVES and MBARS will share the same set of sample holders, and samples will be measured routinely at both spectrometers for the spectra analysis. The ultimate goal is to routinely obtain and analyze the relaxation spectra comparable in coverage to, e.g., dielectric spectroscopy spectra, but with the Q-resolution and high definition sensitivity unique to a neutron scattering probe. BWAVES was strongly supported by the protein research community, which pointed out its unprecedented capabilities for probing hierarchical biological systems characterized by numerous overlapping relaxation processes. The extension of the dynamic range to high energy transfers is highly advantageous for studying protein interactions with solvents in realistic solvation environments. The low-and medium-energy part of the scattering spectra will characterize the protein relaxations, whereas the medium- and high-energy part of the spectra will provide information on the solvent and co-solvent molecules.

During the spectrometer ranking assignment, the panel members vote was split evenly between MBARS and BWAVES. The participants have agreed that both spectrometers should be built at the STS, but the colloid research community suggested that MBARS be built first (Dr. Yun Liu, National Institute of Standards and Technology National Center for Neutron Research/University of Delaware), whereas the protein research community proposed that BWAVES be a first day instrument (Dr. Yang Zhang, University of Illinois). A small sample size, identical for the two spectrometers, was universally appreciated.

The panel recommendations for BWAVES and MBARS could be summarized as follows. While it is to be decided which of the two spectrometers should be constructed first, it is understood that the ultimate goal will be to operate them in tandem for many, if not most, biological and soft matter experiments. Therefore, during the design stage of the STS layout, decisions should be made in such a way as to preserve the space required for successful operation of both spectrometers near the same neutron wavelength of 20 Å. For MBARS, this requires a long-primary flight path (70-80 m) strictly normal to the decoupled moderator. For BWAVES this requires a very short primary flight path (15 m optimal, not to exceed 16 m) facing a coupled moderator.

4.7 INVERSE GEOMETRY SPECTROMETERS FOR CHEMICAL SPECTROSCOPY

Anibal (Timmy) Ramirez-Cuesta (chair), ORNL; Ken Andersen, European Spallation Source; David Banks, University of Tennessee; Jonas Birk, Paul Scherrer Institute; Mark Bowden, Pacific Northwest National Laboratory; Stuart Campbell, ORNL; Yongqiang Cheng, ORNL; Michael Crawford, DuPont Company; Luke Daemen, ORNL; Barbara Evans, ORNL; Thomas Huegle, ORNL; Erik Iverson, ORNL; Jetana Kittisenee, University of Tennessee, Knoxville; John Larese, University of Tennessee, Knoxville; Tyrel McQueen, Johns Hopkins University; Adam Moule, University of California, Davis; Yang Ren, Argonne National Laboratory; Nancy Ross, Virginia Tech; Paul Stonaha, ORNL; Robert Williams, Los Alamos National Laboratory; Zili Wu, ORNL; Haiyan Zheng, Center for High Pressure Science and Technology Advanced Research

The breakout session devoted to "inverse geometry spectrometers for chemical spectroscopy" began with a detailed overview of the proposed concepts, expected performance, and the science case for the JANUS, SPHIINXS, and XTREME-X instruments.

JANUS couples a medium-resolution, broadband indirect geometry spectrometer with a medium-resolution, direct geometry spectrometer. It is aimed primarily at the chemistry community (materials discovery, energy, catalysis). JANUS addresses a number of problems currently plaguing neutron vibrational spectroscopy. First, in direct geometry it is possible to work at low momentum transfer, which is attractive in the situation where recoil is a problem in instruments such as SNS BL-16B, VISION. Second, the Q dependence of the spectrum can be retained, albeit at a lower resolution than, say, SNS BL-17, SEQUOIA, but at a resolution sufficient to identify dispersive modes. Third, high frequency vibrations can be studied at good resolution with the instrument in direct geometry mode. This information complements that obtained in indirect geometry where intensity and resolution are often too low to exploit this part of the spectrum. Fourth, by working at low Q in direct geometry it is possible to work at the higher temperatures the community needs to address certain classes of problems such as catalysis. The use of low Q minimizes the effect of the Debye-Waller factor on the vibrational spectrum, it will open up the use of INS for the study of liquids. Finally, performing measurements with direct and indirect geometry configurations without disturbing or changing the sample represents a major advantage of JANUS.

The breakout session participants were particularly enthusiastic about the JANUS concept in that it would provide the community with a flexible instrument combining two familiar, proven techniques, albeit in a unique combination. The technical specifications were reviewed and met with the approval of all present. Of particular interest was the opportunity to build a chemistry laboratory on a beam line and the possibility of building a “sample changer” of “sample environments” that will make this instrument extremely powerful and unique.

The main reservation expressed by the participants has to do with the fact that the instrument can be operated either in direct or in indirect mode, but not both modes simultaneously. Instrument reconfiguration will be necessary to switch from one mode to the other, which will complicate the beam line design and operation. The corresponding engineering challenge will require the use of substantial resources to design and build JANUS. It was noted that meeting this engineering challenge will force SNS to remain at the forefront of instrument design and construction.

The main conclusion of the discussions centering on JANUS is that the beam line offers a novel, flexible approach at low risk (= proven concepts) and without requiring a "retraining" or development of the user community. As such, the instrument would be productive immediately.

XTREME-X is an indirect geometry instrument for chemical spectroscopy. Its horizontal arrangement of analyzers will enable the use of sample environment equipment (e.g., pressure cells or magnets) that are not usable on inverted geometry instruments with a traditional analyzers configuration. The use of concentric analyzers and the repetition rate multiplication concept will make XTREME-X a high throughput beam line serving the needs of multiple communities of users: magnetism and hard condensed matter, energy, materials and inorganic chemistry. This was perceived as being an advantage, with a concern expressed that careful user management will be necessary to avoid dominance over time of one particular community over the others.

The main focus of the instrument is to expand the range of sample environments available for chemical spectroscopy, particularly with respect to magnetic fields and high pressure while retaining resolution and count rate. The participants felt that this instrument is a most welcome addition that addresses in a timely manner requests made frequently by users over the year. The concept is innovative but presents technical risks.

XTREME-X will focus on small samples (1 x 1 mm^2 to 1x1 cm^2 beam cross section) with a focusing optics system that remains to be specified. This specification was deemed to be adequate by all present. The main reservations revolved around the nature of the focusing optics and the ability to polarize the SNS pulsed beam over the wide range of incident neutron energies (-2 to 500 meV) necessary for instrument operation. Technical investment in these areas will be necessary in parallel with the development of a proposal to develop and implement the XTREME-X concept.

SPHIINXS is a high resolution, broadband spectrometer for neutron vibrational spectroscopy with Q resolution. It is specifically directed at the chemistry/chemical spectroscopy community. SPHIINXS is similar to SNS BL16B, VISION and the LAGRANGE instrument already implemented at the ILL, but retaining Q resolution.

The main advantages of the instrument are (a) the analyzers cover a very large solid angle around the sample (high count rate and large Q range) and (b) Q resolution is retained. Participants pointed out that these features represent clear and distinct advances over VISION when Q resolution is needed.

The technical risks are low to non-existent. The concept was found less exciting than the JANUS and XTREME-X concepts with SPHIINXS providing essentially a "workhorse" to help meet the high demand of neutron vibrational spectroscopy beam time on VISION while offering the extra Q resolution capability to the relevant subset of spectroscopy problems. The specifications were found to be adequate. This is a compact instrument, with a small footprint, excellent performance, with a guaranteed community of followers.

The main question raised by participants concerned the nature (and size) of the sample environment that could be implemented on SPHIINXS.

Summary:

- All three concepts were reviewed from the standpoint of performance, science case, technical feasibility, novelty, and user community impact. All three were found sound and highly desirable with high impact on science and users. All three instruments take advantage of the pulsed nature of the source. No reactor instrument will replace or even compete with them.

- The consensus was that the JANUS and XTREME-X concepts went farther in terms of novel development and extensions of current techniques (JANUS) and access to sample environments that are new to the field of chemical spectroscopy (XTREME-X). SPHIINXS was found to be less exciting and more of an incremental advance in those respects.

- The breakout session participants still recommended the addition of SPHIINXS to the STS instrument suite, noting the extremely high demand on VISION and the fact that neutron vibrational spectroscopy instruments are scarce worldwide while the demand in the context of hydrogen research is growing and likely to remain strong over the next decade and beyond.

- A brief discussion took place regarding the needs for high performance data acquisition hardware and software given the expected throughput of the proposed suite of instruments for chemical spectroscopy. Such developments are already underway with VISION as a test bed. Similarly, the working group believed new approaches to modeling were needed to exploit the data stream that will come out of the new suite of chemical spectroscopy instruments. Such developments are already underway, in part, with VISION. Additional discussions were found to be out of the scope of the breakout session, requiring more time and the presence of more data acquisition/modeling experts to make additional progress.

4.8 IMAGING AND ENGINEERING DIFFRACTION

Andrew Payzant (chair), ORNL; David Anderson, ORNL; Kevin Berry, ORNL; Matthew Connolly, National Institute of Standards and Technology; David Jacobson, National Institute of Standards and Technology; Scott Jorgensen, General Motors Research and Development; Boris Khaykovich, Massachusetts Institute of Technology; Paul Langan, ORNL; Nick Lavrik, ORNL; Jiao Lin, ORNL; Dong Ma, ORNL; Dayakar Penumadu, University of Tennessee; Edmund Perfect, University of Tennessee, Knoxville; Premkumar Saganti, Prairie View A&M University; Harley Skorpenske, ORNL; David Tam, Rice University; Mark Wendel, ORNL; Kenneth Weston, Nucsafe, Inc.; Xingru Yan, University of Tennessee

The community of researchers in the Imaging and Engineering Diffraction breakout session represented a small cross-section of the community who specialize in the use of neutron scattering for the study of engineering materials. The breakout began with a brief overview of the ORNL three source strategy and the specifications for STS and the opportunity for a new class of instruments to support research relevant to materials science and engineering. The instruments under consideration for this breakout session included MENUS, POPCORN, GINI, and there was discussion of other instruments such as SWANS which were relevant to this community. The proposed concept instrument "MENUS" was identified as the highest priority within the engineering/applied materials sciences community.

The primary questions addressed during the breakout session were: (1) What is the vision for science needs in the next decade and beyond; and (2) How to provide a full suite of instruments and capabilities optimized across the three ORNL neutron sources? Within the latter discussion we considered what is adequately covered with existing and planned HFIR and FTS instruments, and what new instrument/science opportunities are opened up by STS?

Imaging instrument concept development projects that have been undertaken at HFIR/SNS to date were reviewed. These included experiments at SNS BL-7, VULCAN and/or SNS BL-3, SNAP, to test specific TOF imaging concepts for the planned SNS BL-10, VENUS, including Bragg Edge studies to elucidate microstructure, texture, and strain, and resonance measurements to enable elemental/isotope composition mapping. The need for continuous development of sample environments to enable *in situ* imaging was highlighted.

Engineering instrument concept development projects that have been undertaken at HFIR and FTS to date were reviewed. These included discretionary time experiments at VULCAN explore texture mapping, an LDRD project that included experiments at VULCAN to test the SWANS instrument concept, an LDRD

project at VULCAN to explore high spatial resolution of strain, composition, and microstructure, and various additional measurements to better understand detector needs and tradeoffs between scintillator and ^{3}He detectors.

Cold Neutron Imaging at HFIR. It was noted that CG-1D, the Cold Neutron Imaging Beam Line, has been tremendously productive and in high-demand, with a rapidly growing community of users. There was universal agreement that it is essential to continue to operate and enhance cold neutron imaging capabilities at HFIR, with increased staffing and improved software tools.

TOF Imaging at SNS (FTS). It was noted that the "VENUS" design is ready, and has been for some time, but as of the workshop date funding was still not yet in place to start construction. There was unanimous agreement that for this community VENUS needs to be built as soon as possible – ORNL is already significantly behind other major facilities (ISIS, J-PARC, Paul Scherrer Institute), and will continue to fall behind until VENUS is operational. It is a challenge to develop a user community based on "proof of principle" experiments run on beam lines like SNS-BL3, SNAP and SNS BL-7, VULCAN when dedicated beam lines are available overseas.

TOF Imaging at SNS (STS). With VENUS not yet under construction, and unlikely to be fully operational before STS development and construction begins, it was agreed that it would be premature to request another imaging beam line for the initial suite of instruments at the STS. However, two interesting concept instruments had been put forward for consideration. The Pinhole (POPCORN) and grating instrument concepts have the potential to enable quantitative phase imaging, with far-field diffraction. Such an instrument would have applications for such diverse topics as batteries, biological tissue, and magnetic domains, and enable high spatial resolution imaging beyond what is presently feasible. It was suggested to consider possibly combining the pinhole and grating concepts into a single instrument with multiple capabilities. It was agreed that these concepts are intriguing but considered not ready for first suite of instruments, and so the participants recommended ongoing proof of concept support to further develop these ideas, possibly at a proposed development beam line at FTS and STS.

Second Generation Neutron Residual Stress Facility (NRSF2) at HFIR. It was noted that HFIR's HB-2B provides important capabilities in mm and sub-mm spatially resolved strain mapping of important engineering materials including steels, aluminum alloys, etc., and has built a unique user community. It is considered essential to continue to operate and enhance thermal neutron strain mapping capabilities at HFIR, with improvements/upgrades including upgrading to 2D detectors, adding radial collimator optics, and enhanced software for data collection and analysis, to continue to support the large class of research that does not require either the unique TOF measurement or the large-sample capabilities provided by SNS BL-7, VULCAN at the FTS.

SNS BL-7, VULCAN. The engineering diffractometer planned at the FTS. It was noted that VULCAN is a world-class instrument, but even after 5-6 years of operation in the user program still needs to be fully built out as planned (i.e., with additional detector banks). Based on recent tests associated with an LDRD project, simply replacing the current wavelength shifting fiber (WLSF) detectors with banks of ^{3}He detectors will provide critical gains in both efficiency and spatial resolution that would greatly enhance the instrument over the current state, and enable studies not presently feasible on the instrument. This is in part due to the WLSF detectors failing to meet the specifications originally anticipated in the instrument design. The participants felt that completing VULCAN to the initial plan has not received enough priority up to the present, and that building out the detector banks should be a priority to ensure the instrument remains world-class.

Multimodal Engineering Instrument at STS. The proposal "MENUS" represents an entirely new high-flux versatile multi-scale engineering beam line which generated considerable excitement from the workshop

participants. Several "proof of concept" experimental results collected at the VULCAN beam line were presented to illustrate the potential of this new instrument. The proposed STS instrument would enable multiscale microstructural characterization with integrated sample environment. MENUS will provide orders of magnitude long wavelength flux and higher spatial resolution than VENUS or NRSF2. With the proposed detector coverage the instrument could determine a full strain tensor in a single measurement, and a full texture orientational distribution function (ODF) with minimal sample reorientations. It would be possible to swap between diffraction mapping and diffracted beam imaging, plus incorporate a transmission detector for imaging or SANS studies. This concept, MENUS, was considered to be the highest priority by the engineering community, and is requested to be included with the first suite of instruments developed and constructed at the STS.

4.9 FUNDAMENTAL PHYSICS

Geoff Greene (chair), University of Tennessee

Ultracold Neutrons and the Neutron Electric Dipole Moment (nEDM) at the STS
The question of whether or not the neutron has a permanent, non-zero electric dipole moment (nedm) remains one of the most important questions in particle physics and is a top priority for the Fundamental Neutron Physics program at the SNS. The goal of the current "nEDM" experiment, which is preparing for installation at SNS BL-13, is to attain sensitivity to a possible neutron electric dipole moment at the level of $3x10^{-28}$ ecm. A measurement at this level could impact one of the critical outstanding questions in cosmology, namely why is there an asymmetry between matter and antimatter in the universe. Notwithstanding the importance of an edm sensitivity at this level, another order of magnitude in sensitivity would in fact be even more compelling. The working group believes that the SNS nEDM experiment will be statistics limited, a more intense neutron source will be of great value.

The nEDM project uses stored UCN in a cryogenic NMR system to search for a possible electric dipole moment. The UCN are produced within the spectrometer that will be located in an auxiliary building that is external to the target building. A large cross-section ballistic guide will transport the cold neutrons to the production volume. The UCN are produced by down-scattering from phonons in superfluid Helium contained within the production volume. The neutron phonon interaction has the characteristic that only neutrons within a narrow spectral band around 8.9Å will be downshifted to the UCN regime.

While a substantial gain in the time integrated total flux from the STS is not expected, it is anticipated that an optimized beam line at the STS could give a substantial increase in the flux of 8.9Å delivered to the UCN production volume. Such a guide system would include a high "m" expanding "horn" placed close enough to the STS moderator to be fully illuminated at 8.9Å. In order to realize such a guide, it is likely that a relatively large penetration in the target shielding would be required.

Of course the prospects for an EDM experiment at the STS will depend upon the progress of the nEDM at BL-13, so it is premature to begin specific design work. Nonetheless, this is an important opportunity and it is suggested that the STS include at least one beam line that incorporates a large cross-section penetration through the monolith shielding. Such a penetration would be very difficult to retrofit and failure to include it in the baseline design would effectively preclude this opportunity.

If the STS included a VCN source, then orders of magnitude higher densities of cold neutrons would be available. While such a VCN source may not be included in the SNS baseline design, provision should be included to allow it as a potential upgrade. As with the guide system mentioned above, failure to include, at least, the provision for such a source will effectively preclude it as an upgrade in the future.

APPENDIX 1. WORKSHOP AGENDA

Second Target Station Workshop
October 27-29, 2015

Tuesday, October 27, 2015		
1:00 p.m.	Workshop Welcome	
1:00–1:20 p.m.	Scientific motivation for the STS	Tennant
1:20–1:40 p.m.	Characteristics of the planned STS	Herwig
1:40–2:00 p.m.	Workshop Charge	Eskildsen
2:00–2:30 p.m.	Summary of Soft Matter Grand Challenge Workshop	Pincus
2:30–3:00 p.m.	Summary of Biology Grand Challenge Workshop	Taylor
3:00–3:30 p.m.	Break	
3:30–4:00 p.m.	Summary of QCMD Grand Challenge Workshop	Broholm
4:00–4:30 p.m.	Summary of Materials Grand Challenge Workshop	Parise
4:30–5:00 p.m.	Charge for Wednesday morning breakout sessions	
5:00–5:15 p.m.	Breakout session preparation (Workshop organizers, program advisory committee and discussion leaders only)	
Wednesday, October 28, 2015		
8:00–11:00 a.m.	Breakout Sessions with breakfast: Scientific drivers for the STS	
Biology	Membranes and thin films, structure and dynamics of membrane systems (joint with Soft Matter). Discussion Leader: David Worcester, University of Missouri	Room C466
Biology	Structure and dynamics of proteins, large complexes, and disordered systems. Discussion leader: David Cowburn, Albert Einstein College of Medicine	Room C152
Soft Matter	Colloids, self-assembled surfactants, charged polymers in solution, polymer networks, hydrogels, nanocomposites and hierarchical systems. Discussion leader: Tonya Kuhl, University of California, Davis	Room AG06
Soft Matter	Dynamics in soft matter, glasses, gels, transport in soft matter, and active soft matter. Discussion leader: Yun Liu, NIST Center for Neutron Research and University of Delaware	Room L183
Soft Matter	Membranes and thin films, structure and dynamics of membrane systems (joint with Biology). Discussion leader: David Worcester, University of Missouri	Room C466
Quantum Condensed Matter Physics	Heterostructured and nanostructured materials. Discussion leader: Charles Majkrzak, NIST Center for Neutron Research	Room AG05
Quantum Condensed Matter Physics	Bulk functional materials and emergent states of matter #1. Discussion leader: Raymond Osborn, Argonne National Laboratory	Room C250
Quantum Condensed Matter Physics	Bulk functional materials and emergent states of matter #2. Discussion leader: Bruce Gaulin, McMaster University	Room C354

Materials, Discovery, Characterization and Applications	*In situ* chemical reactions and catalysts. Discussion leader: Thomas Hansen, Institut Laue Langevin	Tent - SNS
Materials, Discovery, Characterization and Applications	Advanced functional materials. Discussion leader: Tyrel McQueen, Johns Hopkins University	Room C156
Materials, Discovery, Characterization and Applications	Advanced energy materials. Discussion leader: Angus Wilkinson, Georgia Technical University	Room C464
Materials, Discovery, Characterization and Applications	Engineering materials. Discussion leader: David Jacobson, NIST Center for Neutron Research	Room AG07
11:15–11:45 a.m.	Instrument selection at the ESS	Andersen
11:45 a.m.–12:00 p.m.	Charge for afternoon sessions	
12:00–1:30 p.m.	Lunch and Poster Session	
1:30–5:00 p.m.	Breakout sessions: Instruments and techniques ***each group selects ~2 candidates for first STS instruments***	
	Powder Diffraction Discussion leader: Asfhia Huq	Room C354
	Single-crystal diffraction Discussion leader: Bryan Chakoumakos	Room C152
	SANS Discussion leader: Volker Urban	Room C156
	Reflectometry Discussion leader: Gregory Smith	Room L183
	Chopper Spectrometers Discussion leader: Mark Lumsden	Iran Thomas Auditorium
	High-resolution backscattering and neutron spin-echo Discussion leader: Eugene Mamontov	Room C250
	Inverse geometry spectrometers for chemical spectroscopy Discussion leader: Anibal (Timmy) Ramirez-Cuesta	Room C464
	Imaging and engineering diffraction Discussion leader: Andrew Payzant	Room C466
5:15–6:00 p.m.	Breakout session outcome evaluation and consolidation (workshop organizers, program advisory committee and discussion leaders only)	
6:00–8:00 p.m.	Dinner with talk from Paul Langan	
Thursday, October 29, 2015		
8:00–9:40 a.m.	Summaries of Wednesday afternoon breakout sessions	Discussion leaders
9:40–10:00 a.m.	Break	
10:00 a.m.–12:00 p.m.	Town Hall meeting to select 8-10 candidates for initial STS instruments	
12:00–12:45 p.m.	Formation of instrument advisory teams	
12:45–1:00 p.m.	Workshop conclusion	

APPENDIX 2. WORKSHOP WORKSHEETS.

The following worksheets were distributed to workshop participants prior to their arrival as aids to prepare for the breakout sessions.

Worksheet: Scientific Opportunities Provided by the STS

The questions listed below will form the basis for the Wednesday morning breakout sessions. In order to ensure a successful workshop you are encouraged to consider these questions in as much detail as possible ahead of time, and be prepared to discuss them at your session. Feel free to bring completed worksheet(s) and elaborate as much as you want (including figures, etc.). You are also welcome to submit completed worksheets to the discussion leader at the end of the breakout session.

Documentation concerning the STS can be found under "STS Related Documents" at the workshop website (https://public.ornl.gov/conferences/neutrons/STS2015/).

Breakout session title: _____

1. **Describe an important scientific opportunity in your field of research that you would like to address over the next decade**. Please include an estimate of the scientific and technological impact this would have and the chance of success.

2. **Discuss how the characteristics of the STS will benefit the scientific opportunity described above.** The characteristics of the planned STS are available at the workshop web-site under "STS Related Documents"

3. **How will the STS complement the SNS First Target Station and HFIR to facilitate the scientific opportunity described above and/or your current research program.** The three-source strategy is discussed in the "Instruments for Emerging Science" report, p. 10+11.

4. **Are any complementary experimental techniques required in addition to neutrons to address the scientific opportunity described above?** This could be anything that fits within the "Lab on a beam line" concept. Do not include sample environment or software, which are addressed below.

5. **Discuss any auxiliary requirements that are needed to address the scientific opportunity described above.** This may include special sample environment or software (data reduction, analysis, simulations), etc.

Worksheet: Instruments and Techniques

The questions listed below will form the basis for the Wednesday afternoon breakout sessions. In order to ensure a successful workshop you are encouraged to consider these questions in as much detail as possible ahead of time, and be prepared to discuss them at your session. Please complete one worksheet for each type of instrument you expect to use at the STS. You are also welcome to submit completed worksheets to the discussion leader at the end of the breakout session.

Documentation concerning the STS can be found under "STS Related Documents" at the workshop website (https://public.ornl.gov/conferences/neutrons/STS2015/).

Breakout session title/instrument type: _____

1. **Specify the key instrument parameters and characteristics required for your research.**
   Feel free to omit parameters that are not relevant for you and add others if appropriate.
   Please indicate which of these are not met by the current instrument suites at SNS and HFIR.

   Beam/sample size
   Wavelength range
   Q-range
   Q resolution
   Energy range
   Energy resolution

2. **Specify physical parameters and/or requirements for sample environment.**
   This may include e.g.:

   Temperature range
   Magnetic field range
   Pressure (include sample dimensions)

APPENDIX 3. CURRENT AND PROPOSED NEUTRON SOURCES AT ORNL

A3.0 INTRODUCTION

Oak Ridge National Laboratory (ORNL) is home to two powerful neutron sources: the High Flux Isotope Reactor (HFIR), an intense steady-state source, and the Spallation Neutron Source (SNS), the world's most powerful accelerator-based pulsed neutron source. During the past several years, these facilities have dramatically expanded both their science capabilities and capacity to support a diverse user community. These facilities currently represent about half of the U.S. capacity to perform neutron scattering experiments. Continuing investments in new and upgraded instruments at these two facilities, along with on-going improvements in technologies and techniques, will add science capabilities and increase capacity over the next five years.

The 1998 report of the Russell Subpanel[6] defining the technical specifications for SNS included recommendations to design the facility "such that it can be operated at a significantly higher power in a later stage" and to include the "capability of additional targets." Both of these recommendations were incorporated into the original SNS design. The mission need for a SNS Second Target Station (STS) has been recognized by the Department of Energy with approval of Conceptual Design (CD)-0 in January 2009 to "provide an additional target station at ORNL optimized for cold neutron beams." The current STS concept is a short-proton pulse, 10 Hz facility optimized for high peak-brightness, long-wavelength neutron pulses produced by coupled moderators. However, a number of proposed instrument concepts (see Appendix 4) take full advantage of the 10 Hz STS operating frequency but require the sharper neutron pulses provided by a de-coupled, poisoned moderator. Current neutronics calculations indicate that such a moderator can be supported with minimal impact on the coupled moderators.

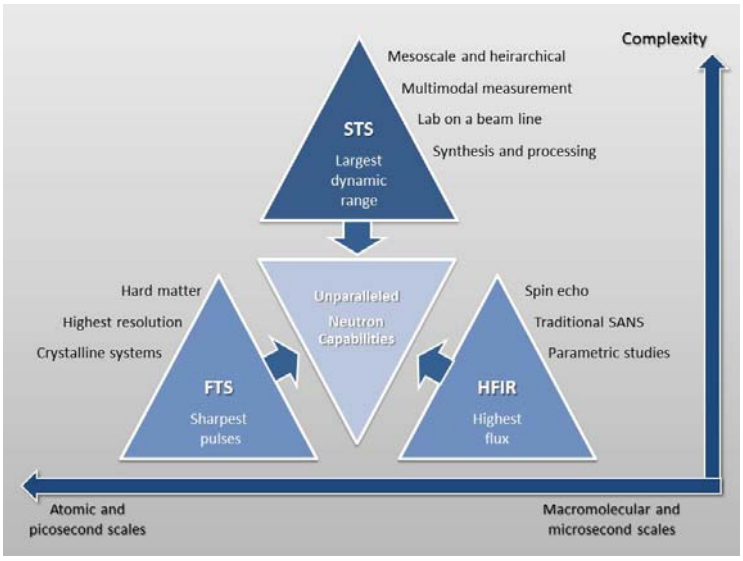

Fig. A3.1. The ORNL three source.

STS will provide the means to address many of the outstanding challenges identified in this 2015 Second Target Station Workshop and the 4 previous workshops, but neutron scattering techniques that are best optimized to different source characteristics are also a key requirement. The cold neutron beams and long repetition rate of STS perfectly complement the SNS First Target Station (FTS) and HFIR. Together these facilities form an unbeatable combination that will give the United States clear leadership in neutron science capabilities for the next 20 years and beyond, allowing it to match or go beyond the capabilities of all existing or planned facilities worldwide. Figure A3.1 summarizes the role of each facility and its strengths and the instrumentation types.

[6] Report of the Basic Energy Sciences Advisory Committee on Neutron Source Facility Upgrades and the Technical Specifications for the Spallation Neutron Source, http://science.energy.gov/~/media/bes/besac/pdf/neutron_source_rpt.pdf (1998).

A3.1 SOURCE CHARACTERISTICS AND STRENGTHS

HFIR

The HFIR cold-source is comparable to the world's best reactor sources and provides the highest time averaged cold neutron flux of the ORNL sources, approximately 10× that of the proposed SNS STS as shown in Fig. A3.2 (a). In addition, HFIR produces approximately 40× the time-averaged thermal neutron flux of the FTS. The guide system delivering neutron beams to the cold instruments in the HFIR guide hall was designed in 1999 and started neutron beam operations in 2006. There have been major advances in neutron guide technology and neutron optics design in the past 15 years which have prompted an assessment of the HFIR neutron guide system. A new guide concept for the HFIR cold source would provide additional instrument end stations and improve neutron beam delivery for current instruments. The workshop discussions included science and techniques that would be best served in a re-optimized HFIR guide hall.

SNS First Target Station

The FTS is optimized for producing the highest wavelength resolution across a wide neutron spectrum. The two de-coupled, poisoned moderators that produce the shortest time neutron pulses and illuminate two-thirds of the SNS FTS neutron scattering instruments are placed in the most favorable positions relative to the Hg target. The two coupled H_2 moderators provide high fluxes of cold neutrons but have much broader time pulses than the de-coupled moderators and are placed in less optimum positions relative to the target, which limits their performance relative to the total number of neutrons they produce. Figure A3.2 (b) compares the pulse widths for the SNS moderators. FTS produces neutron pulses at 60 Hz. The current STS project includes a doubling of the accelerator proton power from 1.4 MW to 2.8 MW with ≈2 MW available to FTS. The neutron scattering instruments and target shielding have all been designed for 2 MW operation, although some

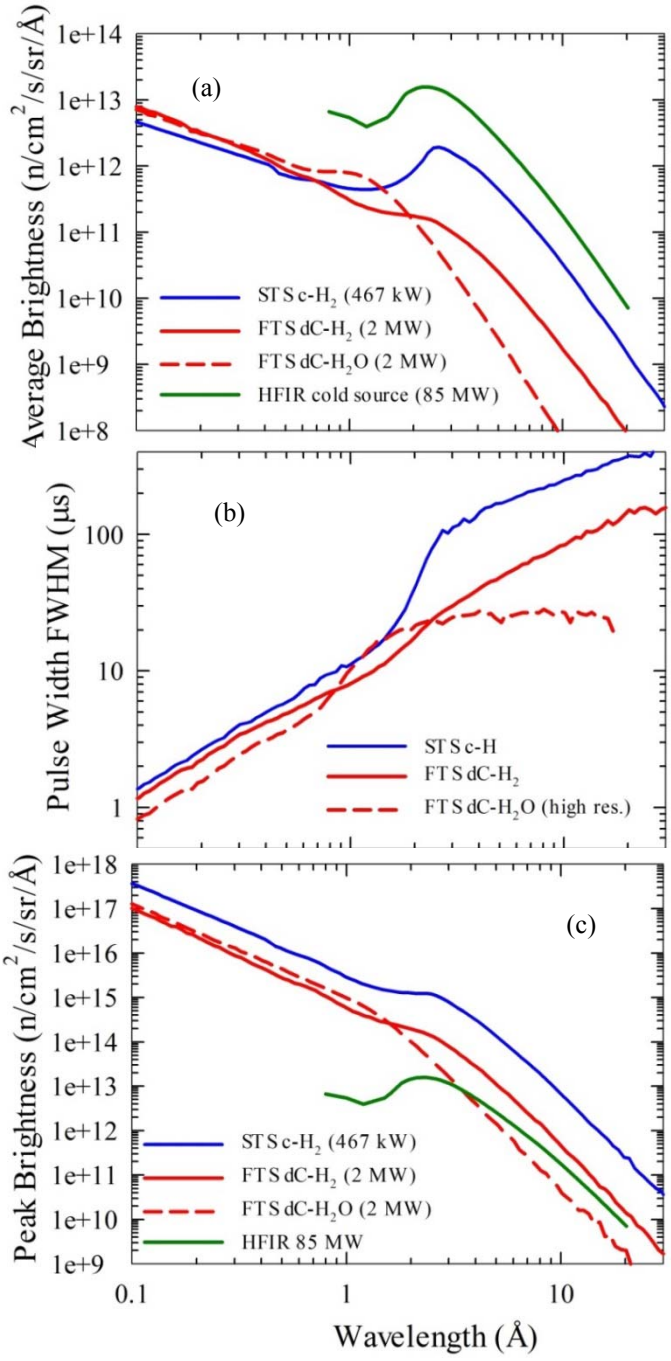

Fig. A3.2. Comparison of ORNL neutron source characteristics. (a) Time-averaged brightness of ORNL neutron sources. The SNS de-coupled and coupled moderators are shown for FTS and STS, respectively. These are the moderators for which each source was optimized. (b) Moderator pulse widths for the FTS de-coupled moderators and the STS coupled moderator. (c) Peak neutron brightness.

target modifications are likely needed because of the increased heat load. The current STS plan calls for operating the two sources in "pulse stealing" mode with five out of six pulses directed to FTS, and the remaining pulse directed to STS. One out of five of the FTS pulses will provide a longer counting time (broader wavelength band as discussed below) because of the missing pulse, but this will be of limited use because the choppers that define this band width cannot be re-set rapidly enough. The chopper systems on FTS will continue to operate as it currently operates, but with one pulse missing out of every six.

SNS Second Target Station

STS is optimized for the highest cold neutron peak brightness, as shown in Fig. A3.2 (c). (Peak brightness is essentially the amplitude at the peak of the neutron time pulse emitted by the moderator as shown in Fig. A3.3.) In complementary fashion to FTS, coupled moderators will be placed in the most favorable positions relative to the target, maximizing their neutron production. Nonetheless, a number of the proposed instrument concepts require a much lower operating frequency than FTS but also require the sharp pulses of the decoupled moderators and would be well-served by the 10 Hz STS. The current STS concept includes three moderators: two coupled moderators of different geometry that are placed in the most favorable locations and a de-coupled moderator illuminating the remaining beam lines. Figure A3.3 shows pulse shapes at select wavelengths for the coupled moderators on both FTS and STS. Reducing the STS moderator dimensions to 3 × 3 cm^2 will improve the peak brightness by an additional factor of ~2 relative to the 10 × 10 cm^2 moderator.

Each of the three current and future ORNL neutron sources has characteristics that are highly desirable for different classes of neutron scattering instruments. The three ORNL facilities will provide a unique opportunity to match neutron scattering techniques and instrument design to the source that delivers the best performance. ORNL will be the only laboratory in the world to provide neutron scattering capabilities optimized across such a diverse set of sources.

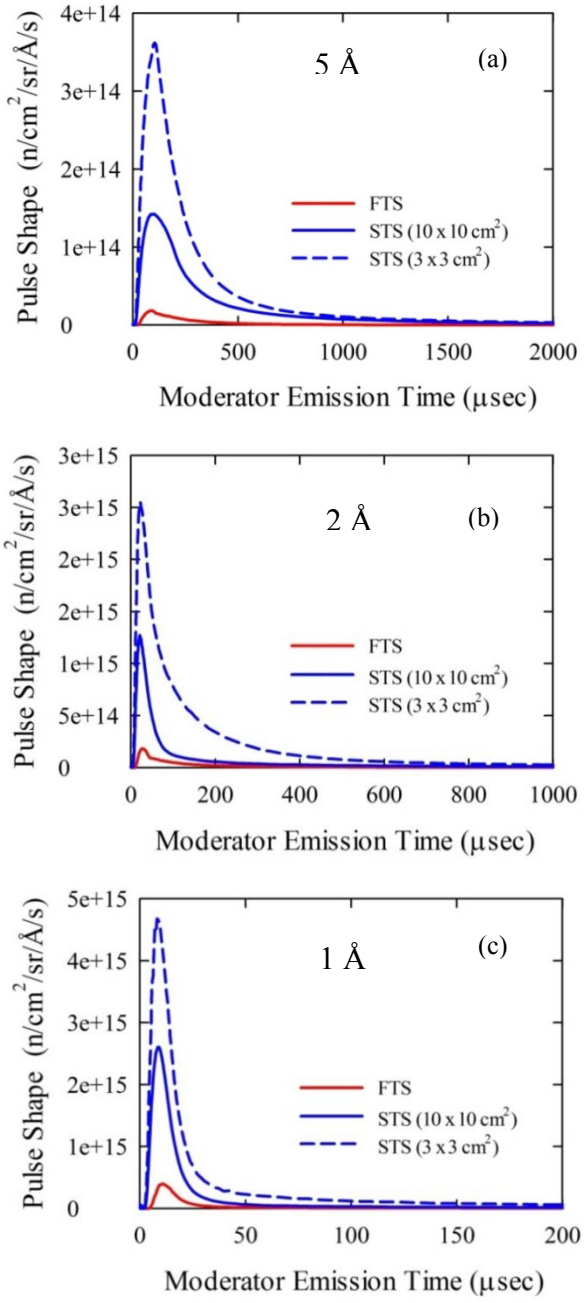

Fig. A3.3. Moderator pulse shapes for coupled moderators at FTS and STS at λ = 5 Å, 2 Å, and 1 Å in (a), (b), and (c) respectively.
Note that the time scale is changing in each plot.

A3.2 STS INSTRUMENT STRATEGIES

Meeting the emerging science challenges of the next decade and beyond requires new paradigms in neutron scattering instrument design and optimization. Performance gains (flux on sample, sample size, resolution, extreme environments in

pressure and magnetic field) on the order of 100 or greater are required (see Section 4 of this report). As discussed above, the current maximum projected source gains of STS relative to FTS are ~10× in peak brightness (Fig. A3.3). The remaining order of magnitude must be achieved in the instrument design or development of associated sample environments. Some of this gain can be realized by use of the newest technologies, particularly in the area of neutron optics. In general, though, STS neutron scattering instruments will inevitably tend toward more specialization and less flexibility. For example, measuring smaller samples may require not only better neutron optics and beam focusing but also an increase in acceptable beam angular divergence (see Appendix 4, the CHESS concept) or development of background reduction technologies (see Appendix 4, the EWALD concept). Following are a few observations about STS instruments and their design:

- The science focus of each instrument must be well-defined because the desired performance gains are likely to push in the direction of less flexible, more specialized, and highly optimized instrument designs.
- Advances in neutron optics must be leveraged. This includes not only advanced guide technology but also development of more sophisticated optics systems such as illustrated by the HFIR CG4D, IMAGINE, instrument and the use of Wolter optics.
- The smaller, high brightness moderators discussed above will enable better optimization of neutron optics systems but likely at the cost of increased mechanical complexity and possible active alignment systems. Particularly in the near moderator regions, care must be taken in the mechanical design of the target monolith to support the higher precision required. It will be important to support a close approach to the moderator of neutron optical systems, 60 cm or less.
- The low, 10 Hz repetition rate of STS will enable the use of much larger bandwidths per pulse, translating to the ability to simultaneously sample much larger length and/or time scales.
- Instrument concepts must mature on a time scale such that they can influence the final choices in moderator and source geometry and neutron spectral characteristics (pulse widths, brightness, and size).
- Development of neutron polarization techniques for use on time of flight (TOF) instruments is crucial because many of the methods commonly used on instruments at continuous sources are not directly applicable. Wide-angle polarization analyzers are particularly important because of the large solid angle detectors' coverage on most TOF spectrometers (see the science cases for CHESS and HERTZ, Appendix 4).

APPENDIX 4. INSTRUMENT CONCEPTS

A number of instrument concepts were developed as part of the science case for the Spallation Neutron Source (SNS) second target station (STS).[Error! Bookmark not defined.] A small number of instrument concepts were contributed in response to a solicitation issued as part of the workshop invitation. These concepts were made available to all workshop participants and were posted on the workshop web site. The concepts specifically considered in the afternoon instrument discussions are briefly described in Table A.4.1, and form the remainder of this appendix

Table A.4.1. Instrument concept descriptions.

Name	Description
Diffractometers	
EWALD – Enhanced Wide Angle Laue Diffractometer Author: Leighton Coates Oak Ridge National Laboratory (ORNL)	Optimized for small macromolecular single crystals
HighResPD – High Resolution Powder Diffractometer Author: Ashfia Huq (ORNL)	Optimized for highest resolution studies of powder samples
NeSCry – Neutron Single Crystal Diffractometer Authors: Huibo Cao, Ovi Garlea, and Bryan Chakoumakos (ORNL)	Optimized for small single crystals with high low-Q resolution, and an emphasis on magnetic structure
VERDI – Versatile Diffractometer Authors: Ovi Garlea and Bryan Chakoumakos (ORNL)	Optimized for magnetic structure studies of both powder and single crystals
MENUS – Materials Engineering by NeUtron Scattering Authors: Ke An, Ducu Stoica, and Andrew Payzant (ORNL)	Optimized for diffraction studies of engineering materials
Spectrometers	
BWAVES – Broad-range Wide Angle Velocity Selector Author: Eugene Mamontov (ORNL)	Indirect geometry spectrometer with high energy resolution and a very broad dynamic range of energy transfers (uses chopper for final energy selection)
CHESS – Chopper Spectrometer for Small Samples Authors: Georg Ehlers and Mark Lumsden (ORNL)	Cold neutron chopper spectrometer optimized for very small samples
HERTZ – High Energy Resolution Terahertz Spectrometer Authors: Georg Ehlers and Mark Lumsden (ORNL)	Cold neutron chopper spectrometer optimized for standard/large samples and relatively high energy resolution
JANUS – Inelastic scattering instrument (INS) Instrument for Catalysis Authors: A. J. Timmy Ramirez-Cuesta, Georg Ehlers, and Luke Daemen (ORNL)	Hybrid indirect/direct geometry spectrometer optimized for irreversible phenomena and *in situ* sample manipulation
MBARS – Mica Backscattering Spectrometer Author: Eugene Mamontov (ORNL)	Indirect geometry spectrometer optimized for ultra-high energy resolution studies (quasielastic neutron scattering)
SPHIINXS – Spherical Indirect Inelastic Crystal Spectrometer Authors: A. J. Timmy Ramirez-Cuesta, Uli Wildgruber, Y.Q. Cheng, and Luke Daemen (ORNL)	Indirect geometry spectrometer optimized for broad-band inelastic measurements of small samples
XTREME-X – Extreme Environment Multi-Energy Spectrometer with Crystal Analyzers Authors: A. J. Timmy Ramirez-Cuesta, Chris Tulk, Bianca Haberl, Mark Lumsden, and Luke Daemen (ORNL)	Indirect geometry spectrometer optimized for measurements restricted to the horizontal scattering plane by extreme sample environments

CAMEA-SNS-STS – INS with high, in-plane efficiency Authors: Jonas O. Birk (Paul Scherrer Institut and Technical University of Denmark) and Henrik M. Ronnow (École Polytechnique Fédérale de Lausanne and University of Copenhagen)	Indirect geometry spectrometer optimized for measurements in the horizontal scattering plane

Multi-Modal Instruments	
HiResSWANS – High Resolution Small/Wide Angle Neutron Scattering Authors: Shuo Qian and William Heller (ORNL)	A combined small angle neutron scattering (SANS)/diffractometer optimized for structural studies from molecular to tens of nanometers
ZEEMANS – High Magnetic Field Beam Line Authors: Garrett Granroth (ORNL), Collin Broholm (Johns Hopkins University), and Andrei Savici (ORNL)	Versatile instrument that integrates neutron spectroscopy, diffraction, reflectometry and SANS with a very high field magnet
Large Scale Structures	
FLOODS – Flux-Optimized Order/Disorder SANS Authors: Chris Stanley and Volker Urban (ORNL)	SANS optimized for highest neutron flux onto small samples with a focus on relatively short length scales, disordered structures and time-resolved measurements.
M-STAR – Magnetism-Second Target Advanced Reflectometer Author: Valeria Lauter (ORNL)	Reflectometer optimized for magnetic studies of small sample areas
WASABI – Wide And Small Angles with Big Intensity Author: Valeria Lauter (ORNL)	Combines measurements of specular reflectivity, off-specular scattering and grazing incidence neutron scattering for measuring 3D structures in films
QIKR – Quite Intense Kinetics Reflectometer Author: John Ankner (ORNL)	Optimized for rapid specular reflectivity measurements from a horizontal sample across a full decade of Q in a single instrument setting
VBPR – Variable Beam Profile Reflectometer Authors: John Ankner and Jim Browning (ORNL)	Horizontal geometry reflectometer optimized to deliver a variable beam profile onto a sample surface as small as 1 mm^2
Imaging	
POPCORN – Polychromatic Phase-Contrast Neutron Imaging Author: Boris Khaykovich Massachusetts Institute of Technology (MIT)	Phase contrast neutron imaging for weak contrast samples
Fundamental Physics	
nEDM@STS – beam line for nEDM measurement Author: Vince Cianciolo (ORNL), Geoff Greene (University of Tennessee, Knoxville/ORNL) and Paul Huffman (North Carolina State University/ORNL)	Beam line to install the neutron electric dipole moment experiment

A.4.1 EWALD – ENHANCED WIDE ANGLE LAUE DIFFRACTOMETER

EWALD is a single crystal diffractometer optimized for the study of macromolecular single crystal samples typically 0.001 mm^3 in volume with unit cells greater than 100 Å on edge. EWALD will open new frontiers in neutron structural biology by enabling x-ray sized crystals to be used for neutron experiments. EWALD will have a performance gain factor of ~75× compared to SNS's BL-11B, MaNDi, at the first target station (FTS). Manipulation of the nuclear spin of H atoms using dynamic nuclear polarization (DNP) holds the promise of an additional gain in signal to noise greater than 100 for hydrogenous samples.

Science Drivers

Visualizing hydrogen atoms in biological materials is one of the biggest remaining challenges in biophysical analysis. While x-ray techniques have unrivaled capacity for high-throughput structure determination, neutron diffraction is uniquely sensitive to hydrogen atom positions in crystals of biological materials and can provide a more complete picture of the atomic and electronic structures of bio-macromolecules. This information can be essential in providing predictive understanding and engineering control of key biological processes—for example, in catalysis, ligand binding, and light harvesting—and to guide bioengineering of enzymes and drug design. By significantly reducing required sample sizes, EWALD (coupled with DNP of hydrogen nuclei) will break through a critical threshold in application of neutrons in biology, opening the door to fundamentally new science:

- Analysis of novel macromolecular structures and rapid structure-activity analysis for the development of inhibitors to human disease targets, engineering enzyme active sites for novel chemistry, and re-engineering enzymes for design properties such as thermal and acid stability for industrial uses.

- Analysis of photochemistry in biology: understanding how hydrogen atoms modulate the site energies and spectral properties of pigment-protein complexes in photosynthetic complexes and the light harvesting machinery that converts light to chemical energy.

- Analysis and refinement of complex active-site electronic structures in metallo-proteins, which are found throughout biology and are used in catalysis, energy capture and conversion, transport and storage, signal-transduction, and genome replication and repair.

Science Requirements

Due to the neutron flux limitations of current neutron sources, neutron macromolecular single crystal diffractometers require samples of at least 0.1 mm^3. EWALD, especially when coupled with DNP, is designed to break this paradigm by the following:

1. The high brightness of the STS coupled moderator provides 50× the neutron flux on sample of MaNDi.

2. Increasing detector coverage by ≈50% relative to MaNDi to approximately 6 steradians

3. The 10 hertz (Hz) operation of STS allows use of the broader pulse widths and higher flux of a coupled moderator by lengthening the instrument to maintain wavelength resolution and still achieve the desired range in d-spacing.

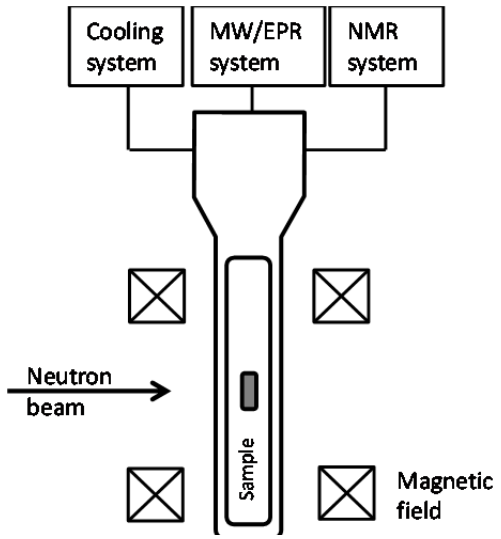

Fig. A.4.1. Schematic view of the EWALD DNP apparatus and its orientation relative to a polarized neutron beam.

4. The instrument will be designed to support DNP which will increase the coherent cross-section of hydrogen nearly an order of magnitude (at the expense of polarizing the incident neutron beam) and improving the signal to noise by suppressing hydrogen incoherent scattering. Polarizing the incident neutron beam will reduce its flux by a factor of two or slightly more.

Technical Requirements

EWALD is a single-crystal diffractometer optimized for macromolecules, with the integrated capability to dynamically polarize the spins of hydrogen atoms in the sample. EWALD will view the 3×3 cm^2 face of the HPCM, face 'b'. At a 90 meter (m) moderator–sample distance, EWALD will have the same wavelength resolution as the much shorter MaNDi instrument that views a decoupled, poisoned hydrogen moderator at the FTS. At the 10 Hz STS pulse rate, the bandwidth per frame, 4.4 Å, is perfectly matched to the most common MaNDi operating mode. The guide system will be curved to avoid the fast neutrons and gammas produced as the protons strike the neutron production target. At least one and possibly two bandwidth choppers will define the wavelength band incident on the sample. Anger camera neutron detectors will be used to measure the scattered neutrons.

A sample that would currently take 10 days of neutron beam time to collect on MaNDi could be collected in only six hours on EWALD enabling multiple data sets to be collected within a single day. Data collection on the radically reduced crystal volumes enabled by EWALD (0.001 mm^3) would increase data collection times to approximately 5-6 days.

Development of DNP is ongoing at ORNL and at other locations in the world. Fig. A.4.1 illustrates the essential elements of a DNP apparatus that includes a low-T dilution refrigerator, a 2.5–5 Tesla (T) superconducting magnet, and a microwave source [2–4 millimeter (mm)]. The requirement to support dynamic nuclear polarization imposes some requirements on instrument design:

- All ferromagnetic materials must be avoided within a radius of at least 2 m from the sample position.
- The sample area must be designed from the outset to support the DNP apparatus that requires specific utilities and room for equipment. (see Fig. A.4.1)
- The detectors must have minimum sensitivity to magnetic fields.

Table A.4.2. Key parameters of EWALD.

Parameter	Description
Moderator	High-peak-brightness coupled moderator, side b
Sample size	1×1 mm^2
Moderator–sample distance	90 m
Sample–detector distance	0.45 m
Wavelength range	2 Å ≤ λ ≤ 8 Å
Resolution	Δd/d = 0.0015
Detector	Anger camera with 1.2 mm spatial resolution

A.4.2 HIGHRESPD – HIGH-RESOLUTION POWDER DIFFRACTOMETER

The High-Resolution Powder Diffractometer (HighResPD) is specified to complement SNS BL-11A, POWGEN, and the proposed RAPID, instruments on FTS. It will provide a high-resolution capability to the U.S. science community with a Δd/d resolution of 0.035%, matching the world's highest-resolution neutron diffraction instruments at the Japan Proton Accelerator Complex (J-PARC) and ISIS.

Science Drivers

Neutron powder diffraction has played a key role in the development and understanding of new, complex materials. HighResPD is optimized to provide the highest resolution of any of the neutron powder diffractometers at the ORNL neutron facilities. This diffractometer has a key role in materials discovery and design; by providing the highest precision examination of atomic-sale structure in topics such as:

- *Ab initio* structure determination from powder diffraction (SDPD): With improvements in instrumentation, algorithm development and enhanced computing power, great strides have been made in *ab initio* structure solution from powder diffraction data. Indexing and determination of space group is the first step in SDPD for which high-resolution data is required. The sensitivity of neutrons to light elements can play a crucial role in the determination of the correct space group, and therefore, the correct interpretation of structure-property relationships.

- Addressing complexity and subtlety in functional materials such as zeolitic solids, piezoelectrics, ionic conductors and others that have very large unit cell volumes and/or subtle structural distortions. This structural complexity is often integral to the useful physical properties of these materials. High-resolution data is needed both to resolve subtle splitting in peaks or reveal subtle features in diffraction line shapes and to resolve an adequate number of Bragg peaks at high Q, where overlap and loss of information are significant issues for large unit cells.

- Magnetic ordering phenomena and magnetic coupling to other physical properties. Magnetic structures can often be extremely complex, requiring high-resolution data to resolve and distinguish long period modulation. A typical example is $BiFeO_3$ where the structure consists of unusually long period modulation of 620 ± 20 Å that was only resolved at very high resolution: I. Sosnowska, et al., *Physica B* 180, 117 (1992)

Science Requirements

HighResPD is optimized to provide the highest resolution of the ORNL neutron powder diffraction suite and has the following requirements:

1. The ability to operate at frequencies as low as 5 Hz in order to provide a wavelength bandwidth greater than 6 Å in a single instrument setting.

2. An integrated suite of sample environment equipment that supports a materials chemistry mission of *in situ/in operando* measurements across a wide range of temperature and pressure, electrochemical cells, and gas handling systems.

3. Acquire refinable data from 0.5 gm sample in on order 1 hour.

Technical Description

Optimized for high d-spacing resolution, HighResPD requires the high wavelength resolution provided by a decoupled, poisoned moderator in combination with a long incident flight path. This instrument will be the longest instrument on the SNS site and uses the 10 Hz repetition rate of the STS to give it a sufficiently wide wavelength band to cover a broad range of d-spacing in a single instrument setting. This instrument will view the cold, para-hydrogen 7×7 cm^2 face of the multi-spectral decoupled moderator. This beam line views the moderator at normal incidence in order to minimize flight path differences for neutrons emitted at different locations on the moderator face. The site geography allows the instrument to be as long as 120 m. The moderator is anticipated to provide a moderator pulse width of 6.8 μsec at a neutron wavelength of 1 Å, giving $\Delta\lambda/\lambda$ of $2.2 \cdot 10^{-4}$ at 120 m, which is sufficient to achieve the desired resolution. The beam line will be straight to provide uniform illumination across the width of the sample.

Optimization might result in a slightly shorter instrument at 100 m, providing a bit more bandwidth in a single frame, 4 Å vs 3.3 Å, to cover a broader range in d-spacing at a correspondingly reduced wavelength resolution of $\Delta\lambda/\lambda = 2.6 \bullet 10^{-4}$. One or possibly two bandwidth choppers will define the incident neutron wavelength band and a T0 chopper will be required. The instrument must preserve the ability to operate effectively at 5 Hz when the broadest wavelength band in a single frame is required. Scaling from the current SNS BL-11A, POWGEN, experience, 1 hour of data collection time is anticipated to be sufficient to obtain a refinable pattern from a 0.5 g sample.

Table A.4. 3. Key parameters of HiResPD.

Parameter	Description
Moderator	Multi-spectral decoupled moderator—cold
Sample size	0.5 to 1.0 cm diameter; 1 to 2.5 cm tall
Moderator–sample distance	120 m
Sample–detector distance	Backscattering and 90°: 2 m Low angle: 3 m
Wavelength range	$0.5 \text{ Å} \leq \lambda \leq 8 \text{ Å}$
Resolution	$\Delta d/d = 0.035\%$
Detector	Low-angle: 0.8 cm diameter linear position-sensitive detector, ^{3}He Backscattering and 90°: to be determined

A.4.3 NESCRY – NEUTRON SINGLE CRYSTAL DIFFRACTOMETER

The cold-neutron single-crystal diffractometer, NeSCry, optimized for studies of small crystal size (0.01–8 mm^3) will accommodate a diverse range of sample environments to enable ultralow temperatures with or without magnetic fields, high pressure combined with low temperature, and applied electric fields. The main distinction of NeSCry is the ability to study small single-crystals, $\geq 0.2 \times 0.2 \times 0.2$ mm^3, with high-resolution at low-Q and superior flux. Considering the ratio in neutron flux provided by STS with respect to FTS, the optimized optical guide, and significantly improved background, the NeSCry is estimated to gain a factor of over 50 in efficiency compared with SNS BL-12, TOPAZ.

Science Drivers

Materials that couple spin, orbital, and lattice degrees of freedom are essential in developing many next-generation technologies. However, many synthesis methods (e.g., flux growth, solvothermal, high pressure, etc.) typically yield small crystal sizes. Neutron diffraction is still the method of choice for elucidating the microscopic magnetic structure of materials and detecting the light atoms in battery or fuel cell materials. Given the increasing complexity of materials (e.g., more elements, low dimensional structures, larger unit cell size, etc.), there is a critical need for neutron diffractometers that have sufficient signal to study much smaller crystals than currently possible. Moreover, currently in the United States, controlled environmental conditions are lacking for single crystal neutron diffraction, which is crucial to detecting emergent phenomena in many areas. In particular, *in situ* studies of crystal growth and ion exchange will be possible, and this will provide new opportunities to study transition and metastable states of a great variety of materials. NeSCry will address topics including:

- Exotic structure and emergent phenomena generally occur with small structural distortion, spin canting, or long period modulation of the nuclear and spin structures simultaneously due to

coupling spin, orbital, electron and lattice degrees of freedom. Their study requires a high Q-resolution and a large Q-range.

- Composite materials that have small lattice misfits are industrially attractive, and in many of these cases, neighboring atoms in the periodic table are also present, necessitating high-Q resolution and neutrons (as opposed to x-rays) (e.g., the phase and microstructure determination of nickel-based superalloys, which are employed in jet engines).

- Energy conversion and storage materials. The large wavelength band provides a great opportunity to study those materials and, more importantly, multiple extreme condition environments are of great importance for *in situ* studies. Single-crystal diffraction can often reveal the true intrinsic physical behavior of materials, which then can be further optimized using nanostructural engineering.

Science Requirements

NeSCry will be designed to provide optimized signal background ratio versatility as a single crystal diffractometer, with or without polarization capability. The instrument requires:

1. Q range of 0.1 – 30 $Å^{-1}$; Q-resolution 0.2 to 0.4%.
2. Sample sizes as small as 0.2 x 0.2 x 0.2 mm^3, volumes ranging from 0.01 mm^3 to 8 mm^3.
3. An option to use polarized incident neutron beam.
4. Adjustable beam divergence from ± 0.5 – 2 degrees.

Technical Description

NeSCry will optimally view the high brightness coupled moderator. NeSCry benefits from the 10 Hz repetition rate giving a large wavelength band per frame, allowing the instrument to be built at 30–50 m from the moderator. This long flight path allows NeSCry to use the broader time pulses of the STS coupled moderators and the significantly higher peak intensity of the neutron pulses, compared with the de-coupled, poisoned moderators typically used on diffraction instruments.

Depending on the choice of instrument length, the instrument will deliver a neutron bandwidth of 7.9–13.2 Å so that the desired Q-range can typically be accessed in a single frame. An elliptical guide system will provide sufficient flexibility to cover a wide range of incident beam divergences. The detector will have high spatial resolution (at least 1 mm x 1 mm) and be located between 0.25 m and 1 m.

Table A.4.4. Key parameters of NeSCry.

Parameter	Description
Moderator	High-peak-brightness coupled moderator, side b
Sample size	as small as 0.2 x 0.2 x 0.2 mm^3
Moderator–sample distance	30–50 m
Sample–detector distance	0.25 to 1 m
λ Range	1.2 Å ≤ λ ≤ 14 Å
Resolution	ΔQ/Q 0.2-0.4%
Detector	High resolution Anger camera or solid state 2D ^{3}He detector

A.4.4 VERDI – VERSATILE DIFFRACTOMETER FOR COMPLEX MAGNETIC STRUCTURES

The cold-neutron diffractometer, VERDI, optimized for studies of magnetism and large unit cell structures will excel by its high-resolution at low-Q and a much-increased flux owing to the high brightness of the source at STS. This instrument will serve for both powder and single crystal studies under extreme conditions of temperature, pressure, or magnetic field. This instrument will be equipped with polarization capability. A VERDI can be expected to have at least five times the count rate of the WISH instrument at ISIS. Its versatility will make it a one-of-a-kind instrument.

Science Drivers

The ever increasing complexity of magnetic systems, which often involve coupled spin, orbital, and lattice degrees of freedom, calls for much improved instrumentation that provides high-resolution at low-Q, high intensity, and reduced extrinsic background. VERDI will meet all these criteria and will be well adapted for in-depth magnetic structure studies as specified below:

- Complex incommensurate structures. VERDI will be optimally suited for studying complex incommensurate structures that arise in multiferroic compounds, one of the new emerging technologies for information processing. The high-resolution and the wide-Q coverage obtained by using a single-frame bandwidth will enable simultaneous characterization of crystal structure as well as local ferroelectric and magnetic properties in these materials.

- Reduced ordered magnetic moments and itinerant magnets. The 4D, 5D, and possibly 6D transition metal oxides are a fertile ground for studies of new magnetic phenomena driven by spin-orbit interaction. The extended nature of the magnetic electrons in such systems requires measurements at small wave-vectors to avoid form-factor suppression of the already weak magnetic signal.

- Magnetization density studies and short-range magnetic correlations. The polarization capability of VERDI will enable studies of the magnetization distribution across magnetic organic molecules as well as studies of the redistribution of electrons accompanying the combined magnetic–crystallographic transitions in martensitic materials. Wide-angle polarization analysis will allow the separation of nuclear, magnetic and nuclear spin-incoherent scattering for unambiguous magnetic diffuse scattering studies.

- Neutron diffraction under extreme conditions. Intriguing new phenomena in quantum materials occur at extreme low temperatures, high pressures, and high magnetic fields. A variety of materials—of which one can name the multiferroics, magnetocaloric materials, frustrated magnetic systems, and magnetic molecular materials—exhibit dramatic changes in their magnetic behavior under high pressures and/or applied magnetic fields.

Science Requirements

VERDI will be designed to provide maximum versatility as a powder or single crystal diffractometer, with or without polarization capability. The instrument requires:

1. The ability to reach low-Q, 0.1 $Å^{-1}$, with extremely low background; Q-resolution 0.2 to 0.4%.

2. Sample sizes 2 x 2 mm^2 to 10 x 20 mm^2.

3. A monochromatic mode supported by a Fermi chopper to improve signal-to-noise as needed.

4. Polarization analysis over 120 degree scattering angle, Helmholtz coils at the sample position are required to support xyz polarization analysis.

5. Adjustable beam divergence (powder: 0.2 to 1° horizontal, 2 to 3° vertical; single crystal up to 1 x 1°).

Technical Description

VERDI will optimally view either the high brightness or high intensity couple moderator, depending on optics design. The smaller moderator will better support the study of small samples. VERDI benefits from the 10 Hz repetition rate giving a large wavelength band per frame, allowing the instrument to be built at 40–60 m from the moderator. This long flight path allows VERDI to use the broader time pulses of the STS coupled moderators and the significantly higher peak intensity of the neutron pulses, compared with the de-coupled, poisoned moderators typically used on diffraction instruments.

It will operate as either a powder or single-crystal diffractometer as desired and will have an integrated polarization capability. The instrument will have a neutron bandwidth of 6.5–9.8 Å so that the desired Q-range can typically be accessed in a single frame. The elliptical guide system will provide sufficient flexibility to cover a wide range of incident beam divergences. This large range of desired divergence to support both powder and single crystal studies will likely require translating guide components. The instrument will include an oscillating radial collimator for background reduction. The ^{3}He detector array will cover 175° in the horizontal plane and extend to ±20° in the vertical. In addition to bandwidth neutron choppers, the beam line is envisioned as incorporating a Fermi chopper that can be translated into and out of the beam to provide a monochromatic beam for studies of diffuse scattering and in select cases to improve signal-to-noise.

Table A.4.5. Key parameters of VERDI.

Parameter	Description
Moderator	High-peak-brightness coupled moderator, side b
Sample size	2×2 mm^2 to 1×2 cm^2
Moderator–sample distance	40–60 m
Sample–detector distance	2.0–3.5 m
λ Range	1.2 Å ≤ λ ≤ 14 Å
Resolution	ΔQ/Q 0.2-0.4%
Detector	0.8 cm diameter linear positive-sensitive detector, ^{3}He

A.4.5 MENUS - MATERIALS ENGINEERING BY NEUTRON SCATTERING

MENUS at the STS will be a transformational high flux versatile multi-scale materials engineering beam line with unprecedented new capabilities. Specifically, in the Q range optimized for low symmetry materials, MENUS has improved flux as much as 250 times higher than SNS BL-7,VULCAN, can deliver, and with the out-of-plane detector coverage, the high spatial resolution residual/*in situ* stress measurement can be performed rapidly at once and *in situ* full orientation distribution function (ODF)/stress orientation distribution function (SODF) can be recorded by rotating the sample around a single axis. MENUS will provide neutron scattering data with high temporal and spatial resolution to materials science and engineering community to tackle and understand lattice strain/phase transition microstructure/texture evolution in three orthogonal directions in complex material systems under combined extreme conditions of stress, temperature, electric and/or magnetic fields, etc. It will open new

scientific opportunities by using neutron scattering for material exploratory, material processing, and material operations.

Science Drivers

The wide Q range coverage in a single frame, the high flux at long wavelength and the novel detector layout make MENUS unique for studying complex structural and functional material behaviors under mechanical, thermal, electrical, and magnetic fields. The rapid data collection rate and the capability to handle large lattice cells or supper lattice structures allow studying phenomena critical to manufacturing and operation of new advanced materials such as:

- Advancing the design of critical engineering materials with supper structure by understanding phase specific stress partitioning.
- Revealing the anisotropic behavior of low symmetry system.
- Understanding the underlying chemistry science in energy materials *in operando*.
- Decoupling the structural and magnetic behavior in functional materials under external extreme fields.
- Unraveling kinetic phase transformation in functional materials and alloys.
- Rapid deep strain scanning in engineering structures with high spatial resolution.

Science Requirements

MENUS needs wide out-of-plane detector coverage to provide three orthogonal structural information at once and large d range coverage of diffraction lines under combined extreme fields; high spatial resolution detector for diffraction imaging; downstream detectors for simultaneous SANS. Exchangeable guides design to satisfy different experimental needs of time resolved or spatially resolved measurements; open sample area to accommodate various sample environments are required.

Sub-second data collection rate and live data streaming/analysis protocol as required by *in situ* or *in operando* observations are needed.

Technical Description

The MENUS instrument will see the high-peak-brightness coupled para-hydrogen moderator (HPCM-c) with a 3x3 cm^2 cross-section at a sample-moderator distance of about 90 m. A single frame at 10Hz will allow bandwidth of 4.4 A, which is equivalent to the SNS BL-7, VULCAN, bandwidth at 20 Hz, and provide 250x flux gain in the lower Q range. Moreover, the neutron pulse contribution to the time of flight (TOF) resolution is estimated to 0.15%, thus, the instrument resolution will match the VULCAN performance in the high-resolution mode. The maximum wavelength range expected to be used is from 1 to 10 A, which corresponds to a d-spacing range of 0.6-6 A in the basic diffraction configuration and can be significantly extended by using low scattering angles detectors. Two instrument configurations are envisioned: high intensity (HI) and high resolution (HR). HI configuration will be dedicated for *in situ* studies of materials under thermomechanical testing and residual stress mapping in complex engineering components. A 1-4 mm^2 sized neutron beam will be delivered at the sample position, with an equal angular divergence of 0.5 deg. in both vertical and horizontal directions; the instrumental resolution is estimated at 0.4% in d-spacing. The HR configuration will provide a 0.2 deg. divergence in horizontal plane, with more flexibility in vertical plane (0.2 to 1 deg.), as well as a tunable cross section of the incident beam. This option is expecting to add more flexibility for studies of functional materials under simultaneous effect of stress, temperature, electric or magnetic fields. An array of detectors will be

positioned at 110 degrees scattering angle, covering about 2 strad. The proposed detector configuration allows to expedite the diffraction analysis by measuring non-coplanar components of the strain; moreover, a complete determination of ODF and SODF in polycrystalline samples can be performed by simply rotating the sample around a single axis (or loading direction under load). Additional detectors with higher spatial resolution will be deployed in the horizontal plane at +/-90 degrees, as well as smaller scattering angles, including a SANS detector. This will allow performing *in situ* simultaneous diffraction and SANS measurements for kinetic phase transformation studies in functional materials and alloys. The HR set-up will include also multi-channel plate (MCP) detectors for imaging in diffraction to visualize the defect distribution and the grain structure in single crystals and coarse polycrystals.

Table A.4.6. Key instrument parameters of MENUS.

Parameter	Description
Moderator type	HPCM-c
Moderator—sample distance	~90 m
Wavelength range	1 to 10 Å (0.6~6 Å in d)
Resolution	Δd/d ~ 0.2% and 0.4%
Sample-detector distance	2 m – diffraction, 5 m – SANS
Detector type	Linear position-sensitive detector ^{3}He, diffraction imaging MCP detectors, and ^{3}He SANS detector in the downstream.

A.4.6 BWAVES – BROAD-RANGE WIDE ANGLE VELOCITY SELECTOR

BWAVES is a small beam size, broadband inverted geometry spectrometer optimized for biological and soft-matter samples that utilizes a novel wide-angle velocity selection device (WAVES)[7] instead of traditional crystal analyzers, for the final energy selection of scattered neutrons. BWAVES alone will cover 5 orders of magnitude in energy transfer, from several μeV to several hundred meV, making it a one-stop instrument for vibrational spectroscopy of biomolecules. The combination of MBARS and BWAVES will cover more than six orders of magnitude in relaxation time. In the quasielastic regime, these two spectrometers will provide access to the same lower-Q range (particularly relevant to soft matter and biology systems) because of identical choice of the scattering angle coverage and the final wavelength of 20 Å.

Science Drivers

INS is indispensable for studying the microscopic dynamics of complex biological and soft matter systems because of a combination of: one, high sensitivity to hydrogen and hydrogen/deuterium selectivity, unmatched by other probes except NMR; two, high energy resolution, far exceeding that attainable in synchrotron x-ray inelastic scattering experiments; and three, sensitivity to the geometry of motions via Q-dependence, which NMR and dielectric spectroscopy do not possess.

However, there are barriers limiting the use of INS for studying biomolecules, including the relatively large incident beam size, which requires large samples, and the limited dynamic range of current neutron spectrometers. The challenge is exacerbated by the complex microscopic dynamics exhibited by soft matter systems, and even more so by proteins, because of the simultaneous presence of vibrational and relaxational processes. This calls for continuous, rather than piecemeal, coverage of energy transfer in a single experiment. Such continuous coverage is provided by inverse geometry spectrometers like SNS BL-16B, VISION, which, however, lack the energy resolution to simultaneously study the quasielastic

[7] E. Mamontov, *Nucl. Instrum. Meth. A*, 759, 83–91 (2014).

signal originating from relaxations in soft matter. BWAVES will address a wide range of topics including:

- Biomolecules in real-life biological solvents. Neutron scattering studies to date have been commonly performed on powder samples with limited hydration. Study of real life biomolecules solvated in aqueous, biologically active media requires an instrument with SNS BL-2, BASIS, like resolution but a much broader dynamic range.

- Microscopic dynamics in complex liquid electrolytes. The research focus for better liquid electrolytes has recently shifted to complex systems such as room-temperature ionic liquids (RTILs). The performance of RTILs in applications is tied to the microscopic dynamics of their cations and anions, which can be quite complex. In the practically important liquid state, the low-energy modes overlap with the quasielastic signal because of both the center-of-mass and side group ion relaxation dynamics, requiring an instrument which can simultaneously measure both quasielastic and inelastic scattering.

Science Requirements

BWAVES is designed to address these challenges by providing:

1. Energy resolution: ≤ 3 μeV (FWHM) at the elastic line.

2. Large dynamic range of energy transfer up to 500 meV.

3. Q-range: $0.06\ \text{Å}^{-1} \leq Q \leq 0.6\ \text{Å}^{-1}$ (in the quasielastic range).

4. Sample size: 0.5 x 0.5 cm^2.

Technical Description

BWAVES requires a low-repetition rate; therefore, it is ideally matched to the 10 Hz repetition rate of STS. This concept relies on development of the WAVES device. Unlike its use on MBARS as an order filter with final energy selected by analyzer crystals, WAVES selects, with high precision, the final energy on BWAVES.

This instrument will view the 3×3 cm^2 face of the coupled, cold para-hydrogen moderator which provides sufficient timing resolution (moderator pulse width) to support the energy resolution desired for BWAVES. To cover the maximum dynamic range of energy transfers in a single STS pulse, the instrument requires a short primary flight path of approximately 16 m. BWAVES will have at least one T0 chopper (two if warranted) to eliminate the prompt pulse and two bandwidth choppers to provide sharp definition of the wavelength band incident on the sample. Vertical

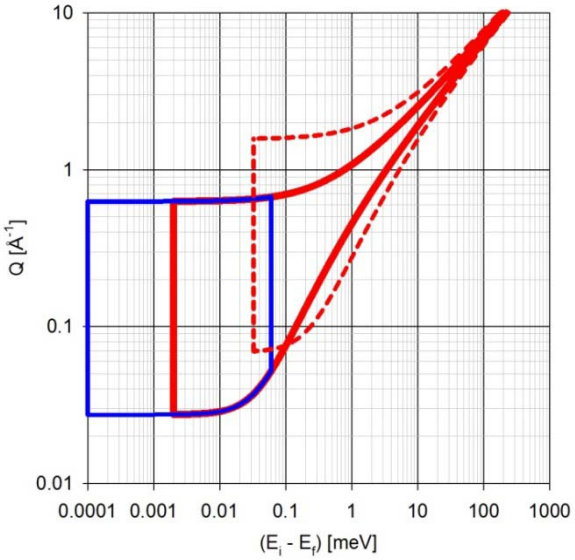

Fig. A.4.2. MBARS and BWAVES momentum and energy space. Blue shows the phase space covered by MBARS and solid and dashed red that by BWAVES when operating WAVES at a final neutron wavelength of 20 and 8 Å respectively.

divergence is likely limited to ±0.5° by the WAVES device, but much broader horizontal divergence could be used. The final flight path can be relatively short so large detector coverage can be readily achieved. The momentum and energy space spanned by MBARS and BWAVES is shown in Fig. A.4.2. Table A.4.6 below lists key parameters of BWAVES.

Table A.4.7. Key parameters of BWAVES

Parameter	Description
Moderator	3 x 3 cm^2 high brightness coupled moderator
Sample size	5×5 mm^2
Moderator–sample distance	16 m
Sample–analyzer distance	0.75 m
Wavelength range	0.4 Å ≤ λ ≤ 23 Å
Q-range	0.06 $Å^{-1}$ ≤ Q ≤ 0.6 $Å^{-1}$ (elastic)
Resolution	3 μeV (FWHM) at the elastic peak
Detector	linear position-sensitive ^3He

A.4.7 CHESS – CHOPPER SPECTROMETER FOR SMALL SAMPLES

CHESS is a chopper spectrometer optimized for very small samples (~ 1 mm – 1 cm) and medium energy resolution, complementary to the higher resolution STS spectrometer, HERTZ. CHESS will take full advantage of the increased peak brilliance of the high brightness STS coupled moderators and of recent advances in instrument design and technology to achieve unprecedented performance in the cold energy range. For small samples, the performance will exceed that of SNS BL-5, CNCS, by a factor of ~200.

Science Drivers

The dynamic structure factor, S(Q,ω), as measured in an inelastic neutron scattering experiment contains information necessary to understand the microscopic interactions in a wide range of quantum and functional materials. However, the traditional large sample size requirement has limited the applicability of this technique and prevented exploration of a great number of materials. CHESS will enable INS on smaller samples than had previously been possible, opening the technique to a broader range of materials such as:

- Small single crystals produced by high pressure synthesis as, for example, the S = 1/2 kagome staircase material β-$Cu_3V_2O_8$.[8]

- Organic superconductors (deuterated) whose synthesis is based on electrocrystallization[9] from which only small single crystals can be obtained.

- Epitaxially grown single crystals that are often used to develop new materials with tailored electronic, optical, or magnetic properties. If such crystals can be grown to micrometer thickness, studies of their excitations using CHESS are feasible.

- Materials under the most extreme conditions which necessitate small sample volumes such as very high-pressure (>40 GPa) which provides an ideal, clean tuning parameter for exploration of quantum phase transitions.

[8] N. Rogado, et al., *J. Phys: Condens. Matter* **15**, 907 (2003).
[9] H. H. Wang, et al., *Chem. Mater.* **2**, 482 (1990).

- Highly absorbing samples where isotopic substitution is not possible such as iridium containing compounds where both stable isotopes absorb neutrons.

Science Requirements

Traditionally, intensity limitations have meant that inelastic neutron scattering measurements could be performed only with relatively large samples (~1 gram of material if it does not contain hydrogen). However, both source and neutron optics advancements now make it possible to break that paradigm so INS can be conducted on the most interesting high quality materials that typically are not available as large (cm sized) single crystals. CHESS offers the following capabilities:

1. A cold neutron direct geometry TOF spectrometer optimized for small samples (~1 mm–1 cm) and medium energy resolution. This will enable mapping excitations over a broad wave vector and energy range for samples with a cross-sectional area as small as 1 mm^2.

2. The instrument will include full three-dimensional polarization analysis to enable separate measurements of multiple components of the $S_{\alpha\beta}(Q,\omega)$ tensor.

3. The low repetition rate of STS will enable simultaneous measurements with multiple incident energies, greatly increasing measurement efficiency particularly in materials with excitations covering a broad range of energies.

Technical Description

Optimized for small samples, CHESS only requires a viewed moderator surface of a few cm horizontally and vertically and is ideally located on beam line 19 viewing the 3×3 cm^2 HPCM face 'c'. The guide entrance will be illuminated with approximately ±3–4 degrees of neutron beam angular divergence. The beam line will be straight and will incorporate a number of choppers to shape the neutron pulse, block the high-energy prompt pulse to minimize background, control the sub-frame durations to support repetition rate multiplication, and monochromate the incident neutron energy. The energy resolution will be tunable in the 2.5–4.5% range, which is typical for direct geometry inelastic instruments. The 10 Hz STS repetition rate coupled with a 25–30 m incident flight path means that all incident energies down to 1 meV can be accessed in the first frame using repetition rate multiplication methods.[10] The neutron beam delivery system must be adaptable to increase beam divergence for small samples to as large as ±4° in either the horizontal or the vertical direction as required. Relaxed energy resolution allows relatively close placement of the detectors to the sample.

It is essential to fully integrate dedicated sample environment equipment into the design of the secondary spectrometer. Extreme conditions in temperature, magnetic field, pressure, strain, and any combination thereof drive the science and must be developed and accommodated within the initial project. Automated sample loading systems for low temperature measurements will also be required on this new generation of high count rate inelastic machines. Also, polarization analysis will be essential for many magnetic experiments because the general science direction is toward systems with smaller moments (spin-1/2) with magneto-elastic effects or excitation continua, whereas traditional methods of isolating magnetic scattering (through temperature variation) are inadequate. These requirements have the following implications:

[10] A special pulse shaping chopper supporting this configuration has been prototyped for the ESS T-REX project. J. Voigt et al., *Nucl. Instrum. Meth. A* **741**, 26-32 (2014).

- All ferromagnetic materials must be avoided within a radius of at least 2 m from the sample position.
- Strict limits must be imposed on the magnetic permeability of the steel of the tank and such components.
- Large coils for magnetic guide fields (several meters in diameter) must be incorporated in the design of the secondary spectrometer.
- There must be at least 50 cm of room between the guide exit and the sample position, and the beam must be shaped such that no diaphragm is needed between the guide exit and sample.
- A collimator between the sample and detector will be required.

Table A.4.8. Key parameters of CHESS.

Parameter	Description
Moderator	High-peak-brightness coupled moderator, side c
Sample size	1×1 mm^2 to 1×1 cm^2
Moderator–sample distance	25–30 m
Sample–detector distance	2.5–3.5 m
Energy range	0.5 meV $\leq E_i \leq$ 100 meV
Resolution	2.5–4.5% variable $\Delta E/E_i$ range; $\Delta Q < 0.05$ Å^{-1}
Detector	1.5 cm diameter linear position-sensitive detector, ^{3}He

A.4.8 HERTZ—HIGH ENERGY RESOLUTION TERAHERTZ SPECTROMETER

HERTZ is a chopper spectrometer optimized for samples as large as 5×5 cm^2, a standard size on many thermal chopper and reactor based spectrometers, with a homogeneous and tunable intensity and divergence profile, complementary to the lower resolution spectrometer, CHESS. The high brightness of the STS coupled moderators combined with advancements in instrument design will enable at least an order of magnitude gain in performance when compared with current, state-of-the-art instruments internationally.

Science Drivers

HERTZ is optimized to provide a large, homogeneous beam to facilitate high-statistical measurements of large volume samples. The cold neutron energy scale is well suited to many critical problems of both experimental and theoretical interest such as quantum magnets, frustrated magnets, and heavy fermion superconductors. One of the strengths of INS is that the measured cross-section is simply related to the scattering function $S(Q,\omega)$, which is amenable to multiple theory or modeling approaches. As such, INS allows for close connections with theory and computation, and neutron data can often provide definitive tests of theoretical models.

HERTZ will provide a critical link between experiment and theory that is essential to enable progress in a number of forefront problems such as:

- Energy related materials including thermoelectrics where detailed microscopic understanding of heat transport derives from measurements of phonon or magnon dispersions and line widths.

- Exploration of competing and coupled orders in multiferroic materials where full understanding of the interplay between magnons and phonons requires detailed measurements of both excitation spectra across the full Brillouin zone with good energy resolution and separation of spin and lattice contributions requires polarization analysis.

- Complex materials in which magnetic scattering features are often weak (due to S = 1/2 entities) or diffuse (because magnetic correlations are short-ranged) using polarization analysis.

Science Requirements

Although CHESS is optimized to enable INS on small samples, there are a large number of problems where one would like to study larger samples with finer energy and wave vector resolution. Such measurements can yield high statistics data providing critical tests for theory and can allow experimental separation of collective modes in complex materials. Consequently, HERTZ is designed to enable the following:

1. A cold neutron direct geometry time-of-flight spectrometer optimized to provide a homogeneous beam as large as 5×5 cm^2. Crystals grown with techniques such as floating zone often reach this size along the growth direction. This instrument will also allow for higher energy (~1% of E_i or better) and wave vector resolution than the CHESS spectrometer.

2. The instrument will be designed to allow full three-dimensional polarization analysis to enable measurements of multiple components of the $S_{\alpha\beta}(Q,\omega)$ tensor.

3. The low repetition rate of STS will enable simultaneous measurements with multiple incident energies, greatly increasing measurement efficiency particularly in materials with excitations covering a broad range of energies.

Technical Description

Optimized for larger samples, HERTZ will view one of the larger coupled moderator faces, either the 3×6 cm^2 HPCM face 'b' or the 5×5 to 7×7 cm^2 face of the HICM depending on the optics design and space optimization. The neutron optics system will be designed to provide individual tuning of neutron beam size and vertical beam divergence at the sample position. The secondary flight path will be long, likely ~5 m, to achieve good energy resolution. The solid angle covered by the detector array will thus be smaller than at CHESS, perhaps ~π ster. The energy resolution defining chopper will have to provide short pulses, ~10 μs or less, and therefore a beam splitter design in the final part of the guide as prototyped at the ISIS LET instrument[11] will be considered. The energy resolution will be tunable in the 0.5–3.0% E_i range. The 10 Hz STS repetition rate coupled with a 25–30 m incident flight path means that all incident energies down to 1 meV can be accessed in the first frame using repetition rate multiplication methods.[12]

Like CHESS, polarization analysis will be essential for many magnetic experiments because the general science direction is toward systems with smaller moments (spin-1/2) with magneto-elastic effects or

[11] R. I. Bewley et al., *Nucl. Instrum.Meth. A*, 637 128 (2011).

[12] A special pulse shaping chopper supporting this configuration has been prototyped for the ESS T-REX project. J. Voigt et al., *Nucl. Instrum. Meth. A* **741**, 26-32 (2014).

excitation continua, where traditional methods of isolating magnetic scattering (through temperature variation) are often inadequate. These requirements have the following implications:

- All ferromagnetic materials must be avoided within a radius of at least 2 m from the sample position.
- Strict limits must be imposed on the magnetic permeability of the steel of the tank and such components.
- Large coils for magnetic guide fields (several meters in diameter) must be incorporated in the design of the secondary spectrometer.
- There must be at least 50 cm of room between the guide exit and the sample position, and the beam must be shaped such that no diaphragm is needed between the guide exit and sample.
- A collimator between the sample and detector will be required.

Table A.4.9. Key parameters of HERTZ

Parameter	Description
Moderator	High-peak-brightness coupled moderator, side b or high intensity coupled moderator
Sample size	1×1 cm^2 to 5×5 cm^2
Moderator–sample distance	25–30 m
Sample–detector distance	4–6 m
Energy range	0.5 meV $\leq E_i \leq$ 100 meV
Resolution	0.5–3% variable $\Delta E/E_i$; $\Delta Q < 0.02$ Å^{-1}
Detector	Linear position-sensitive detector, ^{3}He

A.4.9 JANUS – INS INSTRUMENT FOR CATALYSIS

JANUS is a medium-high resolution, broadband, indirect geometry spectrometer coupled together with a medium resolution direct geometry spectrometer. JANUS is optimized for materials chemistry and catalytic studies involving hydrogenous materials.

Science Drivers

INS provides insight into the microscopic dynamics of molecular species. Neutrons are uniquely sensitive to hydrogen and hydrogenous species due to the large incoherent cross section of hydrogen. Both direct and indirect geometry spectrometers have a role in understanding the dynamics of hydrogen in catalytic reactions. Direct geometry instruments like SNS BL-18, ARCS, and SNS BL-17, SEQUOIA, typically provide good Q-resolution while indirect geometry instruments like SNS BL-16B, VISION, often integrate over Q to get high sensitivity and count rates. Particularly in the case of hydrogen, maintaining good Q-resolution at low scattering angles can provide more detailed information on dynamics that is not degraded by the presence of vibrational overtones and combinations. JANUS combines both approaches into a single instrument, alternately providing good Q-resolution at low scattering angles as a direct geometry spectrometer or maintaining the high sensitivity and count rate at higher scattering angles by integrating over Q like VISION does. An instrument that can do each of these

functions greatly facilitates the study of irreversible phenomena and *in situ* manipulation of samples. JANUS will address topics where the dynamics of hydrogen is of particular relevance including:

- Catalysis: Much of catalysis is concerned with the transfer of hydrogen between reagents and products. Access to the C–H/N–H/O–H stretch region provides a very simple means of identification and is ideally suited to quantification of the species present. The 0–2000 cm^{-1} region is where the details of the catalyst–adsorbate interaction can be discerned and the indirect backscattering detectors provide the good energy resolution needed for this. However, the surface species of interest are often present in low concentration, and good resolution is of no use if there is insufficient sensitivity. This problem is addressed by the direct forward scattering which will provide at least a tenfold increase in sensitivity and possibly as much as a hundredfold increase over the backscattering detectors. The improved sensitivity will also allow industrially important non-hydrogenous adsorbates, such as CO_x, NO_x and SO_x, to be studied for the first time.

- Proton conductors are heavy metal oxides that are hydrated to generate mobile hydroxyls and have considerable potential in intermediate temperature fuel cells. These materials exhibit multiple sites for incorporation of hydroxyls; thus, diffraction studies are only able to provide an average picture of the material, and the crucially important local structure around the hydroxyls is lost. Spectroscopy provides this missing local picture, and INS (in conjunction with first principles modeling) is particularly matched to these needs as the low energy modes enable discrimination between the various possible sites. These modes are often weak or invisible to optical probes. In addition, access to the O–H stretch region is needed to quantify the species present and to discriminate between hydroxyls and water.

Science Requirements

1. An inelastic spectrometer that can provide good Q resolution at low scattering angles $\leq \pm 30$ deg and the ability to provide high count rates and sensitivity by integrating over Q at higher scattering angles.

2. Large dynamic range of energy transfer from -3.0 meV to 500 meV in indirect geometry mode; incident energies up to 300 meV in direct geometry mode.

3. Energy resolution: 1% $\Delta\omega/\omega$; ~150 μeV full width at half maximum (FWHM) at elastic line in indirect geometry mode.

4. Integrated suite of sample environment equipment that provides extreme sample conditions in high pressure, low temperature, and high magnetic field.

Technical Description

This instrument will nominally view 7 x 7 cm^2 water face of the multispectral decoupled moderator. At 20 m from the moderator, JANUS can use neutron wavelengths as long as 19.8 Å in the first frame, covering a wide range of energy transfers simultaneously in indirect geometry operation. JANUS cannot run in both direct and indirect geometry modes of operation simultaneously so the energy selecting choppers directly in front of the sample will need to be parked open when in indirect geometry operation. JANUS will have at least one T0 chopper to eliminate the prompt pulse and bandwidth choppers to provide sharp definition of the wavelength band incident on the sample when in indirect geometry mode. The figure below gives a schematic view of JANUS.

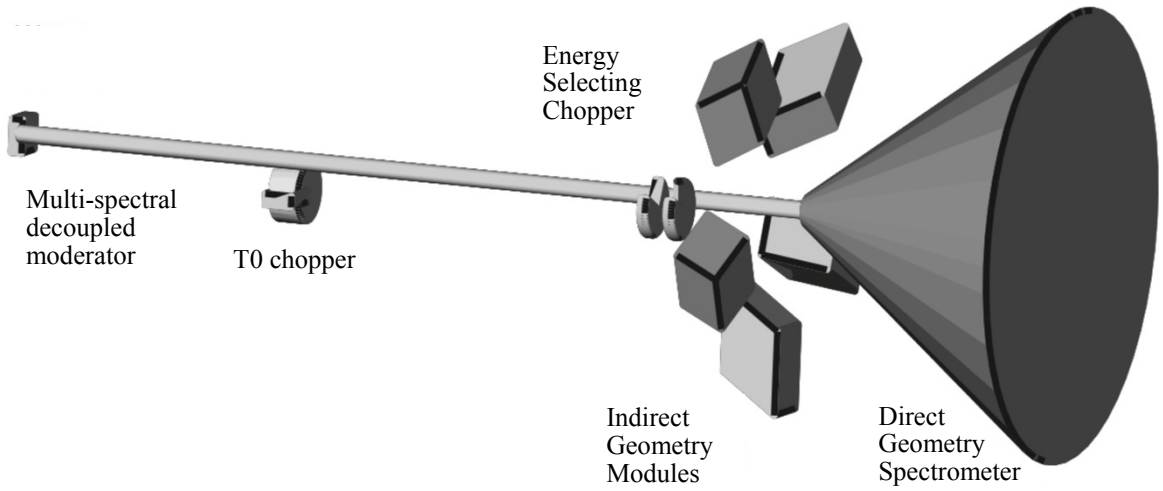

Fig. A.4.3 Schematic diagram of the JANUS spectrometer.

Table A.4.10 Key parameters of JANUS.

Parameter	Description
Moderator	7 x 7 cm^2 water face of the multi-spectral decoupled moderator
Beam size	1×1 cm^2
Moderator–sample distance	20 m
Wavelength range	0.4 Å ≤ λ ≤ 19.8 Å
Resolution	Indirect geometry: 150 μeV (FWHM) at the Elastic peak; Δω/ω ~1% Direct geometry: $\Delta E_{incident}/E_{incident}$ ~1-2%
Detector	Linear position-sensitive ^3He

A.4.0 MBARS – MICA BACKSCATTERING SPECTROMETER

MBARS is a backscattering spectrometer optimized for small samples and very high energy resolution, ≈ 200 neV (FWHM), operating at an elastic neutron wavelength of 20 Å. It is designed for quasielastic neutron scattering (QENS) studies with motions an order of magnitude slower and at a minimum Q three times smaller than SNS BL-2, BASIS. Like BASIS, it will provide a unique combination of high energy resolution and large dynamic range. Data from a 10% scatterer will be collected in 3–10 hours depending on the degree of Q-partitioning desired.

Science Drivers

INS is the only experimental technique that probes not only the time, but also the spatial characteristics of microscopic dynamics on the highly relevant nanometer length scale, through the Q-dependence of the inelastic and quasielastic spectra. As such, this technique is uniquely suited for comparison with and validation of molecular dynamics simulations. The success of BASIS has demonstrated the preference by the scientific community for a combination of high energy resolution and a broad accessible range of energy transfer (dynamic range) for studying microscopic relaxation dynamics. MBARS will measure slow dynamics, including diffusion (local and long-range) and molecular re-orientations across a range of science topics including:

- Protein-solvent coupling. Protein function is strongly affected by interaction with surrounding solvent molecules that exhibit a complex range of dynamics, typically explored as a function of sample temperature. Numerous unresolved controversies in the field largely stem from the energy resolution limitations of current neutron backscattering spectrometers. An order of magnitude improvement in energy resolution will enable unambiguous characterization of the true dynamic properties.

- Ion diffusion in energy materials. QENS can provide detailed picture of ion diffusion in host structures, yielding information such as the diffusion jump length and the residence time between the successive jumps. BASIS has already demonstrated the potential to measure lithium diffusion in battery component materials, but has been limited to high temperature measurements where the instrument resolution can resolve the QENS broadening. Order of magnitude improvement in resolution will enable QENS studies of lithium diffusion under realistic conditions (ambient and slightly below ambient temperature).

- Complex biological and soft matter systems where sample size is an issue. Access to lower Q values and longer relaxation times (to probe larger structural units involved in slower motions) is needed for studying more complex biological and soft matter systems. At the same time, many biological samples are difficult or impossible to synthesize in quantities sufficient to use the traditional (about 10 cm^2) neutron beam cross-section available at backscattering spectrometers.

Science Requirements

MBARS is designed to address these challenges by providing

1. Energy resolution: 200 neV (FWHM)
2. Q-range: 0.06 $Å^{-1} \leq Q \leq 0.6$ $Å^{-1}$
3. Sample size 0.5 x 0.5 cm^2

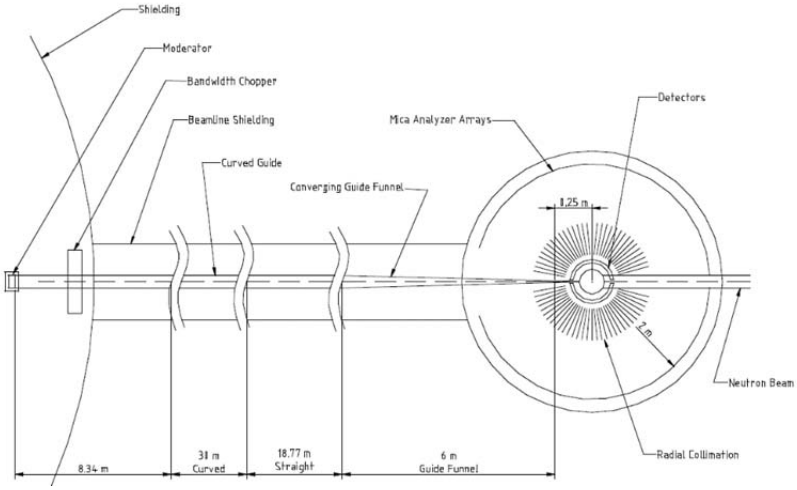

Fig. A.4.4 Instrument layout for MBARS.

Technical Requirements

MBARS requires sharp neutron pulses at a low-repetition rate; therefore, it is ideally matched to a high timing resolution (de-coupled) cold moderator at the 10 Hz repetition rate STS. This concept is nearly identical to an early proposal[13] (see Fig. A.4.4) but proposes an innovative means to filter out high-order contamination from the analyzer crystals using a novel device, the WAVES, under development at ORNL.[14]

This instrument will view the cold, para-hydrogen 7×7 cm^2 face of the multi-spectral decoupled moderator. The neutron guide will be curved to avoid line-of-sight of the moderator and reduce the

[13]H. N. Bordallo, et al., *Nucl. Instrum. Meth. A* 491, 216–225 (2002).
[14]E. Mamontov, *Nucl. Instrum. Meth. A*, 759, 83–91 (2014).

background from prompt neutrons and gammas. The analyzer will be synthetic fluorophlogopite with a 0.3° mosaic (FWHM) in near-backscattering geometry covering a solid angle of 3.7 ster. The neutron guide will deliver at least ±3° of beam divergence in the horizontal direction (higher is acceptable). Divergence in the vertical direction may be limited by use of the WAVES device but will be at least ±0.5°. The beam line will incorporate one or maybe two bandwidth choppers (if sharper open/close transition is required). The table below lists key parameters of MBARS.

Table A.4.11. Key parameters of MBARS.

Parameter	Description
Moderator	Multi-spectral decoupled moderator —cold
Sample size	5×5 mm^2
Moderator–sample distance	75 m
Sample–analyzer distance	2 m
Analyzer–detector distance	1.75 m
Wavelength range	17.9 Å ≤ λ ≤ 23.1 Å
Q-range	0.06 $Å^{-1}$ ≤ Q ≤ 0.6 $Å^{-1}$
ω-range	- 51 μeV ≤ ω ≤ 51 μeV
Resolution	200 neV (FWHM) at the elastic peak
Detector	0.8 cm diameter linear position-sensitive detector, ^3He

A.4.11 SPHIINXS – SPHERICAL INDIRECT INELASTIC CRYSTAL SPECTROMETER

SPHIINXS is a high resolution, broadband indirect geometry spectrometer designed to study small samples. The SPHIINXS concept moves beyond the FTS VISION spectrometer by increasing the analyzer area coverage and retaining Q-resolution.

Science Drivers

Neutron vibrational spectroscopy (NVS) provides insight into molecular structure, chemical bonding, and intermolecular interactions. It is analogous to more common IR and Raman spectroscopies used by chemists but has several well-known advantages including: high sensitivity to hydrogen via its large incoherent cross section; no selection rules; isotopic sensitivity; high penetrating power enabling use of complex sample environments; and quantitative comparison of spectra to theory for both position and intensity. NVS addresses a number of topics in materials chemistry including catalysis, adsorption, storage, separation, and bonding and non-bonding interactions; as well as providing unique insight into the local environments in materials from biochemistry, geochemistry, and condensed and soft matter science. Even with the breakthrough performance of the SNS-BL-16B, VISION spectrometer, a next generation spectrometer is needed that will:

- Be optimized for studying small or weakly scattering samples. This will enable studies of new materials produced through synthesis techniques that can only produce small sample quantities. Smaller samples will also enable use of more complex and extreme sample environments including high pressure.

- Provide both Q and energy resolution by preserving both azimuthal and elevation angle information. Current spectrometers integrate over momentum transfer, averaging out vibrational directional information. Q-resolution will facilitate study of single-crystal samples. Applications include investigation of highly anisotropic local potentials and thermoelectrics where preferential directions can be explored with application of applied electric field.

- Enable rapid data collection for time-resolved, kinetics measurements on time scales of 10s of seconds. One application is monitoring temperature and environmental condition induced decomposition.

Science Requirements

SPHIINXS will address these challenges by providing:

1. A focusing optics system that effectively illuminates a sample area as small as 1 x 1 cm^2; 15x smaller than typically used today.
2. Large dynamic range of energy transfer from -1.5 meV to 1000 meV.
3. Energy resolution: 1% $\Delta\omega/\omega$; ~35 μeV (FWHM) at elastic line.
4. Integrated suite of sample environment equipment that provides control of sample temperature, pressure, gas flow and others. Multiple assemblies must exist that permit measurements on one sample while others are being processed out of neutron beam (e.g. while waiting for chemical reactions to progress).

Technical Description

SPHIINXS requires a low-repetition rate, taking advantage of the 10 Hz frequency of STS to simultaneously cover a large range of energy transfers while maintaining good resolution at the elastic line. SPHIINXS will increase the solid angle covered by the analyzer crystals beyond SNS BL-16B, VISION, by extending the analyzer array in two-theta very much like the geometry employed on more traditional backscattering spectrometers such as SNS BL-2, BASIS, (the vertical slice through the sample position for SPHINKS is shown in Fig. 4.A.5).

This instrument will nominally view 7 x 7 cm^2 water face of the multispectral decoupled moderator. As envisioned, SPHIINXS will use pyrolytic graphite analyzers and requires use of a high-order filter. The analyzers will cover ~10 sr of solid angle, 2.5 x the coverage on VISION. At 40 m from the moderator, SPHIINXS can use neutron wavelengths as long as 9.9 Å in the first frame. SPHIINXS will have at least one T0 chopper (two if warranted) to eliminate the prompt pulse and bandwidth choppers to provide sharp definition of the wavelength band incident on the sample.

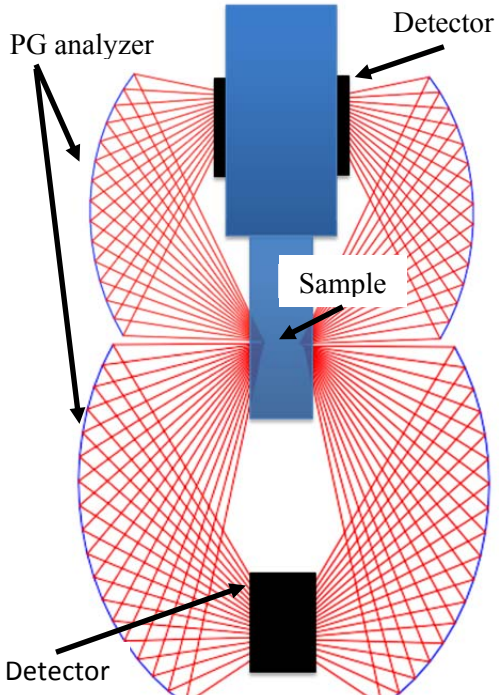

Fig. A.4.5. Sample position for SPHINKS. Vertical slice of the analyzer and detector (black) geometry proposed for SPHIINXS. Red lines indicate paths of scattered and analyzed neutrons.

Table A.4.12. Key parameters of SPHIINXS.

Parameter	Description
Moderator	7 x 7 cm^2 water face of the multi-spectral decoupled moderator
Sample size	1×1 cm^2
Moderator–sample distance	40 m
Wavelength range	0.4 Å ≤ λ ≤ 9.9 Å
Q-range	0.06 $Å^{-1}$ ≤ Q ≤ 0.6 $Å^{-1}$ (elastic)
Resolution	35 μeV (FWHM) at the elastic peak
Detector	Linear position-sensitive ^3He

A.4.12 XTREME-X – EXTREME ENVIRONMENT MULTI-ENERGY SPECTROMETER WITH CRYSTAL ANALYZERS

EXTREME-X is an indirect geometry TOF spectrometer optimized for measuring INS in a horizontal scattering geometry. The choice of horizontal geometry is a necessary consequence of the geometrical restrictions that appear when performing neutron scattering experiments under extreme conditions such as high-pressure or with certain magnetic field designs. The basic concept is to maximize count rates for neutron scattering in the horizontal plane with quasi-continuous analyzer angular coverage of the scattered neutrons. High efficiency will be obtained using banks of concentric analyzers placed behind one other. Each bank analyzes a different scattered neutron energy, which is the indirect geometry spectrometer equivalent of repetition rate multiplication for direct geometry spectrometers.

Science Drivers

Synthesis of innovative materials to address growing energy needs is a key objective in materials sciences. Exploiting extreme environments, notably high temperature and high pressure, has tremendous potential for the synthesis of novel materials with unique, highly useful properties. For example, pressure-induced band-gap engineering may enable the formation of future photovoltaic or superconductive applications from cheap, abundant elements like silicon. Equally, desirable mechanical properties can be engineered such as the immensely increased mechanical strength possessed by diamond and boron-nitride (both high pressure synthesized) or the unprecedented strength-to-weight ratio exhibited by diamond nanothreads recently synthesized at ORNL.[15] The use of specialized, innovative sample environments, radical reduction of background and considerable increase in neutron flux proposed for XTREME-X will ensure that ORNL maintains its status as a world-leader in high pressure inelastic neutron scattering.

INS under high applied pressures or high magnetic fields are routinely used to explore quantum critical behavior and novel phases of matter found in high temperature superconductors, heavy fermion compounds, complex magnetic materials, or other correlated electron systems. Studies at extreme sample conditions such as high magnetic field or ultra-high pressure either necessitate use of small samples or often provide a limited view of the sample from detector locations. Use of the highest vertical magnetic fields limit the view to as small as a few degrees vertically, emphasizing the need to maximize data collection efficiency in the scattering plane. High-pressure is perhaps the cleanest tuning parameter to explore quantum critical phenomena but, of necessity is limited to small sample volumes and limited angular access to scattered neutrons. The efficiency of EXTREME-X in collecting data in the scattering plane will facilitate these studies.

[15] T. C. Fitzgibbons, M. Guthrie, E.-s. Xu, V. H. Crespi et al., *Nature Materials*, doi:10.1038/nmat4088.

Science Requirements

1. A focusing optics system that effectively illuminates a sample area of 1 x 1 mm^2 to 1 x 1 cm^2.

2. Large dynamic range of energy transfer from -2.4 meV to 500 meV.

3. Energy resolution: 1.5% $\Delta\omega/\omega$; ~80 μeV (FWHM) at elastic line.

4. Integrated suite of sample environment equipment that provides extreme sample conditions in high pressure, low temperature, and high magnetic field).

5. Polarization analysis is required to separate magnetic and nuclear scattering.

Technical Description

This instrumental concept for XTREME-X is based on the design of the CAMEA[16] spectrometer (now BIFROST[17]) proposed at the European Spallation Source (ESS). CAMEA is an indirect geometry spectrometer that uses multiple sets of analyzers (one after the other) to select a number of discrete final neutron energies at each sample scattering angle (two-theta). Identical banks of analyzers surround the sample in a semi-continuous fashion. CAMEA was originally envisaged for a long pulse source, but we believe that the CAMEA concept, with some modifications, is significantly better suited for a short pulse source like STS. XTREME-X can be built at a source with a low repetition rate, such as 10 Hz STS. With a frame 100 ms long, it can be positioned at 50 m from the moderator with a direct view of the moderator and still have no frame overlap so that the energy transfer range available is from -2.4 meV to >500 meV and includes the elastic line. The use of solid parahydrogen as a band-pass filter for the neutrons in the secondary spectrometer will remove the higher orders from the spectra. Unlike the CAMEA concept for the ESS, implementation at the STS will provide access to the whole energy transfer range at constant resolution in terms of $\Delta E/E$~1.5%.

This instrument will nominally view 7 x 7 cm^2 water face of the multispectral decoupled moderator. At 50 m from the moderator, XTREME-X can use neutron wavelengths as long as 8.2 Å in the first frame. XTREME-X will have at least one T0 chopper (two if warranted) to eliminate the prompt pulse and bandwidth choppers to provide sharp definition of the wavelength band incident on the sample.

Table A.4.13. Key parameters of EXTREME-X.

Parameter	Description
Moderator	7 x 7 cm^2 water face of the multi-spectral decoupled moderator
Beam size	1×1 mm^2 to 1×1 cm^2
Moderator–sample distance	50 m
Wavelength range	0.4 Å ≤ λ ≤ 8.2 Å
Q-range	0.06 $Å^{-1}$ ≤ Q ≤ 0.6 $Å^{-1}$ (elastic)
Resolution	80 μeV (FWHM) at the elastic peak; $\Delta E/E$ ~1.5%
Detector	Linear position-sensitive ^3He

[16] P.G. Freeman, et al., EPJ Web of Conferences 83, 03005 (2015)
[17] https://europeanspallationsource.se/article/bifrost-prismatic-approach-neutron-spectroscopy

A.4.13 CAMEA - INDIRECT TIME OF FLIGHT SPECTROMETER

CAMEA is a new analyzer-detector concept that has recently been accepted for construction at both a long pulse and a continuous source.[18, 19] It maximizes the number of simultaneously recorded points in the horizontal scattering plane while keeping the count rate in each point at triple axis level. Used in an indirect time of flight geometry on a short pulse source the resolutions can be perfectly matched, making the instrument surpass the already record high in-plane efficiency of the other CAMEA implementations.

Science Drivers

This increase in neutron detection efficiency will bring current fields of neutron spectroscopy to a new level, and will open the powerful technique of neutron spectroscopy to new scientific communities. While ~100 mm^3 samples is currently the practical limit for neutron spectroscopy, CAMEA makes it possibly to study <1 mm^3 samples. Furthermore, being optimized for collecting the maximum number of neutrons scattered in the horizontal plane, CAMEA is superior in combination with large split-coil magnets and anvil-type high-pressure cells. The dramatic reduction in required sample size and the extreme conditions capabilities will enable a series of new possibilities:

- Neutron spectroscopy will become a powerful tool in the discovery of new functionally advanced materials, including search for new superconductors, multiferroics, thermo-electrics, etc.
- Neutron spectroscopy will become possible in up to pressures of >10 GPa both at low temperature for tuning fundamental electronic states of matter and at high temperatures, which will attract the fields of planetary science to use neutron scattering under geo-physically relevant conditions.
- The study of molecular dynamics in biological matter will become feasible.
- Complete mapping of excitation spectra will become possible in higher magnetic fields than currently possible.
- Excitation maps can be measured sufficiently fast that *in situ* and real-time studies become possible with 20 micro-second stroboscopic time-resolution.

Science Requirements

While small samples are often required for extreme environments and also open new fields of science the combination pose several challenges for neutron spectroscopy. Sample environments will often be used for parametric studies which limits the time available for each measurement. Sample environments also produce strong backgrounds that can disturb the weak inelastic signals of small samples. To overcome these challenges an extreme sample environment spectrometer optimized for small samples will require:

- High incoming flux that can be focused on a small sample area.
- High recording efficiency for each measured point in (q,w) space.
- Coverage of as large a fraction of the horizontal plane as possible.

[18] CAMEA ESS - The Continuous Angle Multi-Energy Analysis Indirect Geometry Spectrometer for the European Spallation Source. P G Freeman et al, QENS/WINS 2014.
[19] https://www.lth.se/fileadmin/lth/images/Nyhetsbilder/NORDTEK_Kurt_Clausen.pdf.

- Low inelastic background when large sample environments are mounted.
- Resolutions comparable to other cold medium resolution spectrometers.
- Option for polarization analysis.

Technical Description

Inverse time of flight can expose the sample to the full moderator pulse in a fairly large wavelength band and uses analyzer crystals to reflect most scattered neutrons in a particular point in (q,w) space towards the detectors. This enables the highest possible count rate in the chosen measurement points. To maximize the number of points in the scattering plane simultaneously measured the secondary spectrometer will use the CAMEA principle: A number of concentric analyzer arcs will reflect neutrons to position sensitive detectors below the scattering plane. Together with the new prismatic analyzer concept[20] this will ensure a quasi-continuous coverage of both scattering angle and E_f with a slightly better energy resolution than traditional triple axis spectrometers. The short pulse structure allows easy matching of the primary and secondary energy resolutions. The concept is flexible when it comes to the exact moderator pulse length and frequency but typical numbers could require a 70 m guide. Two choppers will be used to choose and define the desired wavelength band. A ballistic guide will transport a large phase space to the sample position with a high brilliance transfer while keeping the sample out of direct line of sight to suppress the background. It is possible get out of line of sight in 70 m while still maintaining a fairly large horizontal phase space and a large vertical phase space. This matches the angular resolutions of the secondary spectrometer well. Crosstalk shielding in the analyzer tank will ensure that the background stays comparable to that of triple axis spectrometers, while the inverse time of flight will ensure that background neutrons from sample environments will have their slightly wrong flightpath compared to the long primary flightpath and not the short secondary flightpath, thus confining sample environments background very close to the elastic line, unlike direct time of flight spectrometers. Together with the small detector volume and loss of line of sight this enables very low background measurements for inelastic studies.

Table A.4.14. Key parameters of CAMEA.

Parameter	Description
Moderator	Cold
Beam size	1×1 mm^2 to 1×1 cm^2
Moderator–sample distance	35 m
Wavelength range	2 Å $\leq \lambda \leq 8$ Å (1.9 Å wavelength band)
Q-range	0.1 Å$^{-1} \leq Q \leq 2.2$ Å^{-1} (elastic)
Energy Resolution	60 μeV (FWHM) at $E_i=E_f = 5$ meV;
Time resolution	~ 15 μs
Detector	Linear position-sensitive ^{3}He

[20] A Prismatic Analyser concept for Neutron Spectrometers J O Birk et al., Review of Scientific Instruments, 2014.

A.4.14 HIRES-SWANS – HIGH RESOLUTION SMALL/WIDE ANGLE NEUTRON SCATTERING

HiRes-SWANS is a single instrument that combines the features of a modest-resolution neutron diffractometer with a SANS instrument to probe length scales spanning from the interatomic out to tens of nanometers. The instrument takes advantage of the low STS repetition rate and being located as close to the moderator as possible to cover a broad Q-range. A flexible optics system will enable studies in a grazing incidence geometry. HiRes-SWANS is anticipated to have approximately 10x the time-averaged flux at sample as SNS BL-6, EQ-SANS.

Science Drivers

Bulk properties of soft matter derive from phenomena that impact a vast range of length and energy scales. Both bonded and non-bonded interactions produce local structure and function while also driving macromolecular behaviors such as self-assembly and long-range dynamics that ultimately give rise to bulk properties. While the large scale structures forming at 10's of nanometers that arise in soft materials are well-probed by SANS, it is evident that a holistic picture of the structure requires simultaneously understanding interactions at the atomic-level. HiRes-SWANS will measure the evolution of structure and organization across a range of length scales critical to understanding, predicting and ultimately controlling the physical properties of wide classes of materials that are at the forefront of basic and applied research. The instrument will address topics including:

- Understanding the interplay of geometry (e.g., film thickness) and local interactions that drive supramolecular assembly.
- Elucidating the role of interfacial adhesion and chemistry that determine the mechanical strength and functionality of soft/hard composite materials.
- Structure and assembly of hierarchical, complex materials in solution.
- Characterizing process-dependent parameters in 3D-printed polymer composites, including density fluctuations and orientation derived mechanical properties.
- The mechanism of membrane fusion and local lipid reorganization.

Science Requirements

1. Broad dynamic range from 0.01 $Å^{-1} \leq Q \leq 6\ Å^{-1}$; with high-Q resolution, $\Delta Q/Q \leq 0.01$.
2. Include grazing-incidence geometry/optics providing the ability to probe lateral organization as well as structures perpendicular to thin films.
3. Maximum beam size of 1 cm x 1 cm.
4. Open sample area, providing the ability to mount a wide variety of sample environments relevant to soft materials including vacuum ovens, humidity chambers, illumination systems, and simultaneous *in situ* spectroscopies.

Technical Description

HiRes-SWANS could be placed on the high-intensity coupled moderator; however, it could take advantage of the high peak brightness coupled moderator depending on design of the optics system. With a total flight path (moderator-detector) of approximately 20 m, the instrument will have a very broad

wavelength band of approximately 20 Å at the STS 10 Hz pulse rate and be able to probe structures from sub-1 Å to 600 Å simultaneously. The instrument will include a multi-channel bender (with very high-index guide to transmit 0.5 Å neutrons), a focusing optics system, and flexible collimation. The optics design will also be capable of deflecting the beam downward to support grazing-incidence geometry. The low-angle SANS detector will be located 3–5 m from the sample, and the diffraction detectors at angles up to two-theta = 45° will be located approximately 1–1.5 m from the sample. The lowest-scattering angles will require relatively high spatial resolution and must be able to achieve high count rates.

Table A.4.15. Key parameters of HiRes-SWANS.

Parameter	Description
Moderator	High-intensity coupled moderator/High-peak brightness moderator
Sample size	up to 1×1 cm^2
Moderator–sample distance	15–17 m
Sample–detector distance	1.5–5 m
Wavelength range	0.5 Å ≤ λ ≤ 20 Å
Resolution	ΔQ/Q = 0.01
Detector	0.8 cm diameter linear position-sensitive detector, ^{3}He Low-angle Anger camera (1.2 mm resolution)

A.4.15 ZEEMANS – HIGH MAGNETIC FIELD BEAM LINE

Scientific impact, user demand, and two National Academy of Science reports identify neutron scattering in high magnetic fields as a priority area.[21] The enhanced brightness of the STS and progress in high field technology now offer the opportunity for a quantum leap. With continuous fields in excess of 35 T and versatile neutron instrumentation capable of all forms of scattering, the ZEEMANS facility would define the frontier in high field neutron scattering and offer unprecedented new scientific opportunities.

Science Case

The wide-ranging scientific program of the National High Magnetic Field Laboratory (NHMFL) indicates the scientific value of controlling the electronic and nuclear state of materials with magnetic fields in the range from 1 to 100 T. Neutron scattering offers the capability of probing electronic and nuclear structure and dynamics at the atomic scale opens an exciting array of scientific opportunities. The goal is to create the world center for high magnetic field neutron scattering at ORNL in conjunction with construction of the STS. A facility reaching fields beyond 35 T and offering the full range of neutron spectroscopy, diffraction, reflectometry, and SANS with the intensity, resolution, and coverage offered by STS, would have major impact across the whole range of materials based sciences enabling ground breaking experiments that would:

- Expose the structure and dynamics of previously inaccessible quantum matter in correlated metals and insulators;

[21] National Research Council. Committee on Opportunities in High Magnetic Field Science, National Academy of Sciences and National Science Foundation (US), Opportunities in high magnetic field science. 2005, Washington, D.C.: National Academies Press. National Research Council. Committee to Assess the Current Status and Future Direction of High Magnetic Field Science in the United States., National Academy of Sciences, High Magnetic Field Science and its Application in the United States. 2013, Washington, D.C.: National Academies Press.

- Characterize vortex matter in new regimes of high temperature superconducting materials;
- Determine the multiplicity of collective electronic resonances in technologically relevant materials;
- Locate hydrogen in materials relevant to medicine, biology, physical chemistry, and materials science through nuclear spin labeling; and
- Elucidate of the texture and structure of materials during high field processing.

The proposed ZEEMANS facility would thus enable a broad research program and open new directions of inquiry based on the unique magnetic and nuclear interactions of neutrons with materials. Zeemans would create an exciting technological and scientific link between the programs at NHMFL and ORNL's Neutron Sciences Directorate.

Science Requirements

ZEEMANS integrates neutron spectroscopy, diffraction, reflectometry, and SANS with a high field magnet. While such an instrument would be competitive on the FTS, its performance would offer a world leading new capability on STS. By leveraging the highest brightness moderator and the low repetition rate ZEEMANS will deliver performance estimated to be ~20 × SNS BL-12, TOPAZ, and 40 × SNS BL-14B, HYSPEC, for single crystal diffraction and spectroscopy respectively. ZEEMANS requires a sample environment integrated into the high field magnet design capable of controlling the sample temperature from 50 mK to 1,000°C.

Technical Description

ZEEMANS is best located on the high intensity coupled moderator and because of the significant infrastructure required for the magnet facility will be optimally placed on STS BL-1. The beam line will be curved and may include a bender to avoid a direct line-of-sight view of the moderator. It will incorporate a number of neutron choppers and adjustable optical components (the last 5 m of the guide system) so as to tailor the neutron beam for individual scattering techniques. The instrument will include the capability to provide a polarized neutron beam and to perform analysis of the scattered beam polarization. A previous National Science Foundation (NSF) funded project resulted in a conceptual and engineering design for the superconducting magnet system that provides a head start for ZEEMANS.[22] Fig. A.4.6 shows the concept for the detector vessel and magnet that was developed in that project.

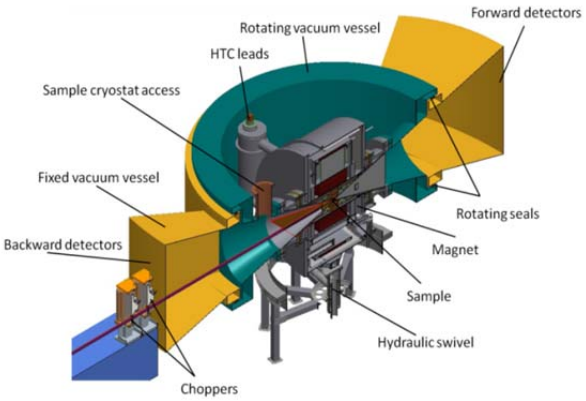

Fig. A.4.6 Schematic diagram of the ZEEMANS spectrometer.

While the current world leading 25 T facility at the Helmholtz Zentrum Berlin is based on a resistive magnet that requires mega-watt power and cooling systems, advances in high Tc technology now indicate a fully superconducting 35-40 T magnet system is possible. For this field range, the magnet will

[22] A. T. Savici and G. E. Granroth, SNS Technical Report, SNS-NSSD-TOF-TR-0002-R00 (2009); G. E. Granroth, et al., in ICANS XIX, 19th meeting on Collaboration of Advanced Neutron Sources; A. T. Savici, et al. *J. Phys.: Conf. Ser.* 251 0120573 (2010).

inevitably define the geometry of the instrument and it will be the main technological challenge. It will furthermore require significant specialized infrastructure in the form of a dedicated helium liquefaction plant and specialized sample environment systems to cool and rotate the sample within the high field. Ongoing magnet development and prototyping work is needed to enable the construction of ZEEMANS as a day one instrument on the STS. ZEEMANS will deliver record-breaking scientific capabilities and through an ongoing partnership with the NHMFL, define state of the art in ultra-high field neutron scattering for the foreseeable future.

Table A.4.16. Key parameters of ZEEMANS.

Parameter	Description
Moderator	High-intensity coupled moderator
Sample size	Maximum: 2×2 cm^2
Moderator–sample distance	60 m
Sample–detector distance	5 m
Inelastic: Energy range	10 meV ≤ E_i ≤ 200 meV
SANS and diffraction: λ-range	1Å ≤ λ ≤ 10 Å
Inelastic resolution	$\Delta E/E_i$ range between 1 and 15% depending on E_i and chopper settings
Detector	8 mm linear position-sensitive detector, ^3He

A.4.16 FLOODS – FLUX-OPTIMIZED ORDER/DISORDER SANS

FLOODS is a TOF SANS optimized for highest neutron flux onto small samples with a focus on relatively short length scales and disordered structures as well as time-resolved measurements. High flux is obtained with high neutron beam divergence at relaxed minimum Q and Q-resolution. In low-resolution mode, FLOODS will provide >10^9 neutrons/second across a 10 mm^2 sample which is ≈1000x higher flux than the current HFIR CG-3, Bio-SANS. In high-resolution mode, FLOODS will have a minimum Q and Q-resolution similar to SNS BL-6, EQ-SANS, but with an order of magnitude higher count rate.

Science Drivers

In general, FLOODS will enable studies of any low contrast and/or weakly scattering samples. The increased neutron flux also improves the time-resolution for kinetics measurements. A particular area of benefit is intrinsically disordered proteins (IDPs). This protein class is shifting the structure-function paradigm in biology as it becomes clear that IDPs, or intrinsically disordered protein regions (IDRs), are highly prevalent in the human proteome (50% of all human proteins are either wholly disordered or contain disordered regions) and essential for function in many biological processes. Many proteins possess IDRs that exhibit heterogeneous, dynamic conformations that are influenced by their environment (e.g., pH, ionic strength, extent of molecular crowding, cellular localization, etc.) and interactions with multiple cofactors, substrates, and regulatory partners. Neutrons can greatly contribute to advancing this challenging area of research because of their unique ability in probing the heterogeneous conformations of disordered systems, in particular disordered regions of proteins. FLOODS will have sufficient beam power and neutron flux required to extract a very low intensity signal from small volume biological samples and will address topics such as:

- Establish relationships between disorder and function in IDPs and proteins with IDRs - A particular challenge with IDPs is that many become unstable with increasing concentration,

leading to undesired precipitation. Furthermore, concentrations can be studied that more closely approach *in vivo* conditions.

- Rational drug design - Many critical-functioning and disease-relevant proteins are difficult to prepare in sufficient quantities for a conventional SANS measurement. For example, numerous drug targets are membrane-associated proteins that typically have low expression yields.

The high flux of FLOODS will also enable time-resolved studies including:

- Monitoring amyloid protein aggregation kinetics; it is a challenge to identify and characterize the earliest formed transient species that are believed to be the most toxic.

- Observing the kinetics of phase transitions that drive phenomena in polymer science including phase separation, gelation, and self-assembly.

Science Requirements

The study of small volume, low-concentration samples and time-resolved kinetics requires an instrument with the highest neutron flux and the following characteristics:

1. A relaxed Q-resolution, $\Delta Q/Q$ ~20 – 50 % with a minimum Q of at least 0.1 $Å^{-1}$.

2. The ability to operate in a more conventional SANS mode with a dynamic range of at least 0.01 $Å^{-1} \leq Q \leq 0.5$ $Å^{-1}$.

3. A neutron beam with flexible optics able to focus on samples from 0.1 mm^2 to 10 mm^2.

4. Sample environments optimized for time-resolved experiments including stopped-flow and continuous-flow devices to support controlled in-beam mixing. The small beam focus will enable use of microfluidic devices.

Technical Description

With its focus on illuminating small samples with the highest neutron flux, FLOODS will optimally view the 3 x 3 cm^2 face of the high brightness coupled moderator at STS. With a total flight path of moderator to detector of 20 m, FLOODS will have a dynamic range in wavelength of 19.8 Å at the 10 Hz repetition rate of STS. FLOODS will include a multi-channel bender (and possibly a T0 chopper as well) to reduce instrument backgrounds as far as possible supporting the study of very small samples. The optics system will be adjustable, able to focus the neutron beam onto a sample as small as 0.1 mm^2. In high flux mode, the relaxed beam divergence of 2 deg (FWHM) implies that a minimum scattering angle (2θ) of ≈8 deg is required to maintain $\Delta Q/Q$ at 50% as the resolution is dominated by the beam divergence. Q_{min} under these operating conditions will be <0.044 $Å^{-1}$ at the longest wavelength, 19.8 Å, accessed in first frame operation. Adjustable collimation can reduce the beam foot print on the detector and reduce $\Delta Q/Q$, allowing for a more conventional SANS set up.

With a focus on small coherent scattering cross sections in samples that typically have high incoherent background from hydrogen (an even deuterium), methods for suppression of incoherent scattering will be extremely valuable. Methods that should further be investigated for potential suitability include: (a) choppers that remove in background from inelastic scattering (i.e., thermalization of cold neutrons in hydrogen-rich samples); (b) dynamically polarized hydrogen; and (c) spin-polarization/analysis. All of

these methods have specific limitations and drawbacks, and their suitability for FLOODS needs further research and development.

Table A.4.17. Key parameters of FLOODS.

Parameter	Description
Moderator	High-peak brightness moderator (3 x 3 cm^2 face)
Sample size	0.1 mm^2 to 10 mm^2
Moderator–sample distance	17 to 18 m
Sample–detector distance	2 to 3 m
Wavelength range	0.5 Å ≤ λ ≤ 20 Å
Resolution	variable ΔQ/Q; 20 – 50%
Detector	0.8 cm diameter linear position-sensitive detector, ^3He

A.4.17 M-STAR – MAGNETISM-SECOND TARGET ADVANCED REFLECTOMETER

M-STAR is a polarized neutron reflectometer optimized for studies of magnetism and structure in magnetic heterostructures. It will define new limits in nano- and meso-science, spintronics and kinetics studies for materials a few atomic monolayers thick to complicated prototype device-like systems with multiple buried interfaces having small lateral dimensions of only several millimeters. M-STAR will cover a simultaneous wide range of momentum transfer for kinetics studies. The combination of high brightness of the STS source with an advanced optics design is anticipated to provide a gain factor ≈200 over the magnetism reflectometer on FTS.

Science Drivers

M-STAR will address a range of science topics, including topological heterostructures, multifunctional oxide heterostructures, domain dynamics (switching and relaxation), multiferroics, and self-assembled magnetic heterostructures. Many of these exhibit unusual physical properties that are important for science and technology and represent recent key innovations. The availability of high performance polarized neutron reflectometry is vital for understanding magnetism in these systems that include:

- A revolutionary new generation of heterostructures has emerged based on integrating topological insulators (TIs) with conventional materials. Proximity with a ferromagnetic insulator (FI) allows the TI surface states to experience ferromagnetic interactions with symmetry breaking at the interface. Examining dual-proximity effects by introducing ferromagnetic order onto the surface of TI thin films is realized by using ultra-thin FI in heterostructures.

- Multifunctional oxide heterostructures exhibit unusual physical properties that represent recent key innovations from both the fundamental and device application viewpoints. Epitaxial thin films of ferroelectric and ferromagnetic oxides are anticipated to find application in low-energy consumption devices. Particular interest is on the room temperature magnetoelectric multiferroic, $BiFeO_3$, exchange coupled to a ferromagnet. The nature of exchange coupling and mechanisms of the voltage control of ferromagnetism under dynamic conditions are topics to be addressed.

- *In situ* studies of kinetics and relaxation processes (domains and re-magnetization process in nanostructures and multilayers) require a broad spectral range and a higher flux combined with complex sample environment. Emergent interface magnetization in several novel interface states is expected to be weak, so these measurements require high statistics up to large Q.

Science Requirements

The studies described above need a polarized reflectometer optimized for samples with lateral dimensions as small as several millimeters.

1. Qmax: ~ 0.4 $Å^{-1}$; Q-range in a single instrument setting: 0.01 $Å^{-1}$ < Q < 0.2 $Å^{-1}$ (at 5 Hz).

2. Sample sizes that range from 2 x 2 mm^2 to 20 x 20 mm^2.

3. Polarized beam with polarization analysis and an un-polarized beam option.

4. Integrated complex sample environments with an extended temperature range of 3 K < T < 750 K, magnetic field -5 T < H < 5 T, electric field E up to 1MV/cm, pressure and light. Many of these conjugate fields should be simultaneously controlled. Some of the conjugate fields should be variable at a rate of 10-100 kHz.

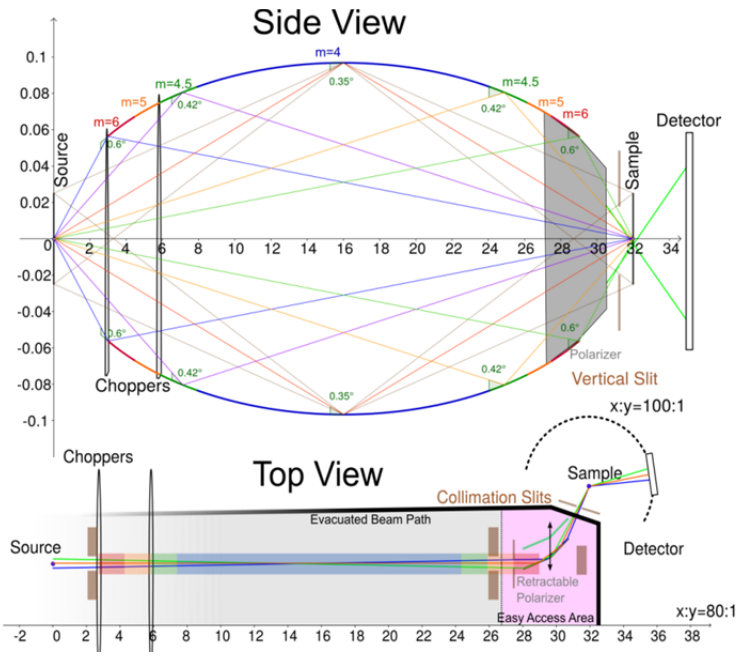

Fig. A.4.7 Schematic diagram for M-STAR.

5. Many complex magnetic systems exhibit high saturation fields and their study requires a superconducting solenoid magnet with a hollow bore to suppress the background. The ability to apply magnetic fields must be integrated with many other sample environments including pressure cells and microwave cavities requiring field uniformity on order a few percent over their relatively large cross-sections ≈100 cm^2.

6. Low background will be provided with the frame overlap mirror and a reflection polarizer.

Technical Description

A proposed concept for M-STAR could be placed on the high intensity coupled moderator or possibly the 3 x 3 cm^2 face of the high peak brightness coupled moderator depending on final optics design. The sample position will be optimized between 20 and 32 m from the moderator to the best trade between the wavelength band and the intensity provided by the focusing optics. With an additional 2 m from sample to detector, M-STAR will reach a minimum wavelength band of 11.6 Å in the first frame. Kinetics studies will require the ability to operate at 5 Hz (suppressing intervening source pulses), doubling the wavelength band accessed. At least two bandwidth choppers will be needed to define the wavelength band and provide the flexibility for 5 Hz operation. The sample geometry could be either vertical or horizontal. M-STAR requires a 50×50 cm^2 detector with 2 mm x 2 mm spatial resolution. The use of polarized neutrons requires special attention to controlling magnetic materials in the vicinity of the instrument and places an additional requirement for minimal magnetic field sensitivity of the detector. M-STAR proposes an optics design that focuses the neutron beam at the sample with relatively high vertical divergence enabling use of small samples and kinetics studies. The focusing optics concept is comprised of elliptical mirrors (as seen in Fig. 4.A.7).

Table A.4.18. Key parameters of M-STAR.

Parameter	Description
Moderator	High-intensity coupled moderator or 3x3 cm^2 High-peak brightness moderator
Beam Size	Variable illuminating samples as small as 2 x 2 mm^2 to as large as 20 x 20 mm^2
Moderator–sample distance	~20 - 32 m (depending on final optics design)
Sample–detector distance	1-3 m variable
Wavelength range	1 Å $\leq \lambda \leq$ 40 Å
Resolution	$\Delta Q/Q > 0.02$
Detector	2D position-sensitive detector, 2 mm x 2 mm vertical spatial resolution

A.4.18 WASABI –WIDE AND SMALL ANGLES WITH BIG INTENSITY

WASABI is a versatile instrument for simultaneous measurement of specular reflectivity, off-specular scattering, and grazing incidence neutron scattering (GINS), the latter comprises both small angle neutron scattering (GISANS) and grazing incidence diffraction (GID). Three-dimensional structures in soft and hard matter films will be probed on multiple length scales from nanometers to tens of microns. WASABI is expected to have a gain in count rate >x200 (x10 from moderator & bandwidth gain; x20 from focusing optics) as compared with the SNS BL-4A, Magnetism Reflectometer, for specular and off-specular reflectivity measurements.

Science Drivers

Functionality often arises at the mesoscale, where defects, interfaces, and non-equilibrium structures are formed.[23] Reflectivity measures scattering along the surface normal of the film and is related to the depth variation of chemical and magnetic structure. Off-specular scattering and GISANS arise from lateral inhomogeneities and provide information on two drastically different length scales determined by the resolution and the neutron coherence lengths. Off-specular scattering measures lateral inhomogeneity with a length scale ~0.1-10μm. GISANS measures the sizes and shapes of heterogeneous materials over lengths scales as large as ~100 nm. GINS establishes a direct and precise correlation between local interfacial characteristics and global physical properties. Challenges in mesoscale materials to be addressed with GINS include:

- Vertically aligned nanoscale architectures in which either the functionality or structure changes across the film depth. Examples include designing and tailoring functional oxide materials with exceptionally high ionic transport and systems such as lipid rafts in model bio-membranes.

- Topologically protected spin textures in memory technologies for development of novel materials that can mediate skyrmions.

- Exchange-coupled composite elements comprising soft and hard layers, e.g. for permanent magnet applications.

[23] *From Quanta to the Continuum: Opportunities for Mesoscale Science*, a report from the Basic Energy Sciences Advisory Committee (2012); http://science.energy.gov/~/media/bes/pdf/reports/files/OFMS_rpt.pdf.

- Rheology studies of liquids and soft matter.
- Origin of flexomagnetism (i.e., influence of the strain tensor on magnetic structure).
- Self-assembly of colloids at charged surfaces.
- Influence of charged surfaces on magnetic phase separation in films.
- Influence of ion implantation (which is non-uniform with depth) on phase separation in oxygen dispersion strengthened steel and on stabilization of skyrmions.
- Response of confined ferrofluids to magnetic field.

Science Requirements

The studies described above need a new approach to instrument design that incorporates GINS as an optimized requirement rather than an add-on to a conventional reflectometer.

1. Q_z-range in a single setting 0.01 $Å^{-1}$ < Q < 0.10 $Å^{-1}$, Qy and Qx variable of (neutron wavelength λ, sample-detector distance and detector dimensions)
2. Sample sizes that range from 1 – 25 cm^2.
3. Flexibility for both unpolarized and polarized beam operation (with optional polarization analysis).
4. Low background (no direct view of the source from the sample position),
5. Integrated complex sample environments with an extended temperature range of 3 K < T < 750 K, magnetic field H <+/- 5T, electric field E, and pumped light optics.

Technical Description

WASABI could be placed on the high intensity coupled moderator or possibly the 3 x 3 cm^2 face of the high peak brightness coupled moderator depending on final optics design. The low repetition rate and high brightness of the peak of STS is ideally designed for new generation GINS with polarized neutrons. The low repetition rate allows for a broad wavelength band necessary to obtain the wide Q range at one incident angle and to perform experiments at constant geometry. The optics design will maximize the intensity for

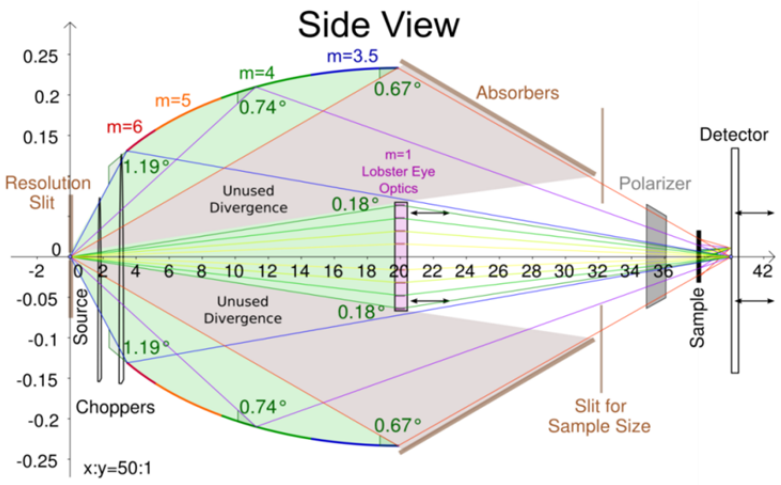

Fig. A.4.8. Focusing optics with focus at the detector position.

GI-SANS (design illustrated has the sample at 38 m from the moderator). With an additional 2 m from sample to detector, WASABI will reach a maximum wavelength of 9.9 Å in the first frame. One or possibly two bandwidth choppers will define the wavelength band. The sample is vertical with horizontal scattering geometry. WASABI requires a 50×50 cm^2 detector with 1.5 mm horizontal and 2-2.5 mm vertical spatial resolution.

A proposed concept for WASABI utilizes a novel optics design that focuses the neutron beam at the detector position enabling the use of large samples in GISANS geometry. The focusing optics concept is a combination of elliptical mirrors and lobster eye optics (see Fig. A.4.8). Table A.4.19 lists key WASABI parameters.

Table A.4.19. Key parameters of WASABI.

Parameter	Description
Moderator	High-intensity coupled moderator or 3x3 cm^2 high-peak brightness moderator
Moderator–sample distance	30-40 m (depends on final optics design)
Sample–detector distance	1 – 2.5 m
Wavelength range	2 Å ≤ λ ≤ 26 Å
Resolution	Adjustable: $0.01 \leq \Delta Q/Q \leq 0.1$
Detector	2-dimensional position-sensitive detector, 1.5 mm horizontal, 2-2.5 mm vertical spatial resolution with count rate of 0.5–1 M counts/s and a peak count rate of 5–10 M counts/s. The detector must have a broad dynamic range of ~10^7

A.4.19 QIKR – QUITE INTENSE KINETICS REFLECTOMETER

QIKR will be a versatile multipurpose reflectometer featuring horizontal sample geometry and a broad "single-shot" Q-range for structural and kinetic studies of solid, solid/liquid, and free liquid surfaces and interfaces. QIKR will collect specular reflectivity data at a single (θ, $\Delta\lambda$) instrument setting over a full decade of Q (e.g. 0.02 $Å^{-1}$ < Q < 0.20 $Å^{-1}$). In addition to radically simplifying data collection and reduction, "one-shot" measurements eliminate the 60–90 s required to change chopper phases and move motors between Q bands on existing SNS reflectometers, enabling broad-Q specular reflectivity to be measured in seconds or less. This purely kinematical advantage, coupled with improved STS cold flux, can yield ×100 improvements in time resolution.

Science Drivers

Neutron reflectometry covers a broad spectrum of science involving the growth, self-assembly, structure, and interactions of a wide variety of thin film materials and impacts many core areas of polymer, chemical, biological, and materials science. Because the advanced thin film materials of the future will be increasingly complex, there is an urgent and ongoing need to develop high performance neutron reflectometers to elucidate their structures over length scales range from 1 nm to 1000 nm.

The challenges to be met in soft condensed matter and the life sciences are as wide ranging as the topics investigated. While the sensitivity of neutrons to structural features offers a significant advantage in many types of multicomponent system, the recent literature shows a clear trend toward following time-dependent processes. These processes include, but are not limited to:[24]

[24] H. Wacklin and A. Vickery. "ESS Instrument Construction Proposal–FREIA" (2014).

- Self-assembly of surfactants, polymers, and proteins at solid and liquid interfaces.

- Rearrangement processes in thin films: polymer interdiffusion, inter-layer movement, lipid flip-flop, and annealing/drying/exchange/wetting processes in composite films such as those used in photovoltaic applications.

- Encapsulation and release of components in plastics, polymer blends, drug delivery and implant materials, and chemical and biological sensors.

- Switchable materials that undergo structural changes in response to external chemical, mechanical, electrical, or magnetic stimuli.

- Surface reactions that involve changes in film structure or chemical composition; e.g., enzyme catalysis, oxidation or other film degradation reactions, receptor-ligand binding, drug-target interactions, surface functionalization, etc.

Science Requirements

Kinetic studies like those described above are infeasible with any of the FTS reflectometers because of the need to use multiple instrument settings to collect data over the necessary Q-range. Requirements for a kinetics reflectometer include:

1. The ability to measure a full decade in Q (e.g. from 0.02 $Å^{-1}$ < Q < 0.20 $Å^{-1}$) in a single instrument setting.

2. Sample sizes that range from 1 – 15 cm^2.

3. Option for polarized beam and polarization analysis.

4. Wet chemistry lab adjacent to the instrument to support sample preparation.

5. Fully integrated suite of sample environments including a Langmuir trough, environment chamber, potentiostat and others.

Technical Description

QIKR could be placed on the high intensity coupled moderator or possibly the wider viewed face (3 x 6 cm^2) of the high peak brightness coupled moderator. The sample position will be placed as close to the moderator as possible to maximize the Q-range sampled in a single frame, approximately 13.5 m. At a total flight path of 15 m to the detector, the instrument will reach a maximum wavelength of 26 Å in the first frame of operation. Q_{min} of 0.02 $Å^{-1}$ is reached with a beam incident on sample at an inclined angle of 2.37 deg. Reaching Q_{max} = 0.2 $Å^{-1}$ at this same angle requires 2.6 Å neutrons which are at the peak of the spectral distribution of the moderator. QIKR requires a 20×20 cm^2 detector with 1 mm pixel resolution capable of a sustained count rate of 0.5–1 M counts/s and a peak count rate of 5–10 M counts/s. As the entire reflectivity curve is captured in a single instrument setting, the detector must have a dynamic range of 10^7. The neutron guide will be curved or possibly will incorporate a multi-channel bender and may employ elliptical focusing in the horizontal direction. One bandwidth neutron chopper (or possibly two) will define the incident neutron wavelength band.

Table A.4.20. Key parameters of QIKR.

Parameter	Description
Moderator	High-intensity coupled moderator
Beam Size	Variable as large as 1.5×3 cm^2; illuminating flat samples from 1 – 15 cm^2
Moderator–sample distance	as short as 13.5 m
Sample–detector distance	1.5 m
Wavelength range	2.5 Å ≤ λ ≤ 26 Å
Resolution	$\Delta\lambda/\lambda$ <0.01
Detector	^{3}He 2-D position-sensitive detector (if possible)

A.4.20 VBPR – VARIABLE BEAM PROFILE REFLECTOMETER

VBPR is a horizontal geometry neutron reflectometer capable of delivering a variable beam profile onto a sample surface as small as 1 mm^2 without the use of apertures in the immediate sample position. The instrument will take advantage of the pulse characteristics and brightness of STS combined with advanced focusing optics to deliver a broad wavelength band at high fluence. This permits the acquisition of an extended Q-range from a small sample area using a single instrument setting, enabling the study of small samples or small areas of a larger sample.

Science Drivers

Interest in surface and interfacial phenomena continues to increase across diverse scientific areas ranging from biology to geoscience. When coupled with isotopic substitution or complicated sample environments, neutron reflectometry (NR) remains a method of choice in the study of interfaces. However, current interest is shifting to samples that do not meet the traditional neutron reflectivity sample criteria of a large, homogeneous surface area. Examples include patterned or graded surfaces used to understand layer conformation and its effect on surface properties, solid-state diffusion over short length scales, hybrid (organic/inorganic) materials of technological interest with limited lateral dimension or heterogeneous surface structure, or materials in extreme environments and include topics such as:

- Nanopatterned surfaces formed by e-beam lithography have been proposed as platforms to investigate structure such as the conformation of suspended soft-surface coatings or protein conformation at the surface of a suspended lipid bilayer.[25] The ability to probe such systems on a millimeter length scale will eliminate the need to produce large patterned surfaces and open new areas of research.

- Formation of the solid-electrolyte interphase is critical to the performance and safety of energy storage materials. It can be difficult to obtain a uniform electric field over large surface area electrodes, leading to lateral inhomogeneity in layer formation. The ability to define a small beam profile on the sample makes it possible to select specific areas or eliminate the need for large-area electrochemical cells altogether.

- The study of diffusion processes over short length scales (~ nm) is a developing area of research in energy storage, nanostructured, and semiconductor materials. *In situ* NR can play a major role in the study of such systems by using stable isotope substitution (e.g., ^{6}Li/^{7}Li in energy storage materials) and multilayered film configurations. VBPR will enable the use of much smaller

[25] G. Smith, et al., *Nano Research* **6**, 784 (2013).

samples eliminating concern over use of costly isotopes and more significantly, improve time resolution by improving the response time of heating and cooling samples.

- In general, large beam profiles average over the entire surface of the sample, losing information regarding lateral inhomogeneity. The ability to focus the beam to as small as 1 mm^2 will allow the user to "raster" a sample, effectively measuring variations in the scattering length density profile as a function of lateral position on the sample. This could allow NR measurements of nontraditional materials such as naturally occurring minerals or samples deposited onto irregular surfaces.

Science Requirements

The key requirement is for a reflectometer with an optics system designed to deliver a small, variable beam footprint) onto a horizontal sample without need for beam defining apertures very close to the sample for samples as small as 1mm x 1mm. Gains in beam intensity over an unfocused case should be ~30x to permit the measurement of reflectivity curves with $R<10^{-6}$ in fractions of an hour (see reference 29). To capture the reflectivity with a minimal number of measurements for ease in data analysis, the instrument must sample a broad wavelength band to maximize the measured Q-range ($\Delta\lambda>12$Å). The sample area must accept standard sample environments and provide for translation in the plane of the sample to raster the finely focused beam for areal studies and provide precise alignment for small area samples.

Technical Description

Optimized for small beam footprints, VBPR will view the 3 x 3 cm^2 highest brightness coupled moderator at STS. Like the kinetics reflectometer, it is desirable to place the sample position as close to the moderator as possible to maximize the Q-range sampled at a single instrument setting. However, the elliptical guide design that provides precise control over the beam profile may dictate placing the sample somewhat further from the moderator reducing the Q-range. For example, the elliptical focusing system proposed for the ESS Estia[26] is approximately 30 m long with the detector an additional 6 m from the sample. At this distance, a 13 Å bandwidth is available at the 10 Hz operating frequency of STS. Slow, kinetic studies will require twice this wavelength band and the chopper system must be designed to allow 5 Hz operation by eliminating intervening pulses. The instrument will require at least one (or more likely two) bandwidth choppers to define the wavelength band.

Table A.4.21. Key parameters of VBPR.

Parameter	Description
Moderator	High-peak brightness coupled moderator (3x3 cm^2 face)
Beam Size	Variable to provide a footprint on sample from ~ 1 mm^2 to several hundred square millimeters
Moderator–sample distance	30 m
Sample–detector distance	2 - 6 m (final distance is TBD)
Wavelength range	2.5 Å ≤ λ ≤ 25 Å (5 Hz) 2.5 Å ≤ λ ≤ 12.5Å (10 Hz)
Resolution	$\Delta\lambda/\lambda$ <0.05
Detector	^{3}He 2-dimensional position-sensitive detector (1 mm resolution)

[26] https://europeanspallationsource.se/estia-truly-focusing-reflectometer

A.4.21 POPCORN -- POLYCHROMATIC PHASE-CONTRAST NEUTRON IMAGING

POPCORN is a novel neutron-imaging instrument, which would allow quantitative measurement of the phase changes of a partially coherent neutron beam passing through samples. The instrument would be used to measure mesoscopic structure of materials and devices, from batteries to biological tissue samples, by measuring their neutron refractive index in 3D. The samples will be illuminated by a broadband, pulsed polychromatic beam through a small aperture, of about 0.2 mm diameter, or less, creating a partially coherent beam. The imaging will be done in the time-of-flight mode and the phase delay will be calculated from the intensity variation at the detector a few meters downstream from the sample.

Science Drivers

POPCORN will enable studies of any weakly absorbing samples as devices, which have inhomogeneous structure on the length scale of 1 micron. Specifically, it will be suitable for measuring extremely small variations in thickness of thin films or material or isotope content in thin-film samples. Particular applications include

- Energy materials and devices, such as batteries
- Thin films and devices
- Biological tissue
- Films and membranes under external stress or strain
- Porous substances and metallic foams

Technical Description

Neutrons are waves, having both an amplitude and phase. When a partially coherent wave interacts with a sample, the phase changes due to refraction in the sample material. Phase change is proportional to the refractive index, i.e. even weakly absorbing samples affect the phase of the beam. However, the phase is too fast to be detected directly. Phase differences are computed from intensity measurements with the help of the transport-of-intensity equation (TIE). The TIE is symmetric with respect to the sample-detector distance and neutron wavelength. Therefore, by scanning the wavelength one can extract neutron phase variations quantitatively, leading to direct measurements of neutron refractive index of weakly-absorbing samples. The energy-resolved pinhole method has been demonstrated with x-rays and in visible light.[27] POPCORN will implement this strategy for neutrons at the STS by utilizing the TOF method. In the pinhole phase-contrast imaging, the partially coherent beam is created by using a small pinhole aperture. The sample is placed at a distance from the pinhole (~ 0.5 m), while the detector is place a few meters downstream from the sample. (The recently developed grating phase-contrast method results in higher signal rates than the pinhole method, because the source size is larger, but the grating requires a quasi-monochromatic beam to achieve high contrast. Therefore, to use the broad energy band available at SNS, the gratings should change or move with at the neutron pulse frequency. Most importantly, the grating method is not suitable for quantitative measurements of the phase, but only relative phase changes, because it is not sensitive to the 2π periodicity of the phase.) The pinhole method measures the phase change and thus the refractive index, directly. The TOF pinhole method at the STS would use neutrons of the broadest possible range of wavelengths for quantitative phase reconstruction, thus using both the high flux and the pulse structure most effectively.

The resolution of the phase measurement is determined by the beam coherence (aperture size) and the TOF resolution ($\Delta\lambda/\lambda$). The spatial resolution must reach ~ 1 – 10 μm level to achieve the science

[27]Gureyev, T.E., Mayo, S., Wilkins, S.W., Paganin, D., Stevenson, A.W., 2001. Quantitative In- Line Phase-Contrast Imaging with Multienergy X Rays. *Phys. Rev. Lett*. 86, 5827–5830. Waller, L., Kou, S.S., Sheppard, C.J.R., Barbastathis, G., 2010. Phase from chromatic aberrations. *Opt. Express* 18, 22817. doi:10.1364/OE.18.022817

objectives. Such resolution is achievable because the beam divergence and a significant distance between the sample and the detector result in large geometrical magnification. One possibility to reach very high phase resolution is by using focusing mirrors with equal focusing distance, a 4*f* optical system, between the sample and the detector (Waller et al., 2010). POPCORN would utilize the high brightness of the small STS moderators. The optimization of the neutron guide system will be needed to create a very bright small source. One possibility is to use long (~ 40 m) focusing guides to concentrate the beam from a 30x30 mm moderator surface to create a very bright partially coherent source.

Table A.4.22. Key parameters of POPCORN.

Parameter	Description
Moderator	High-peak brightness; small size
sample size	thin films (1 - 100 μm thick)
Field of view	10 x 10 mm

A.4.22 NEDM@STS – A NEUTRON ELECTRIC DIPOLE MOMENT (EDM) EXPERIMENT AT THE SECOND TARGET STATION

An experiment to measure the neutron's electric dipole moment is currently being mounted on SNS BL-13, Fundamental Neutron Physics beam line, of the FTS (nEDM@SNS). That effort incorporates many novel techniques and has the goal of improving the current best measurement statistical precision by two orders of magnitude and reducing the systematic errors significantly below that, such that the precision is simply determined by the available number of neutrons. If the current effort succeeds in reaching a statistics-limited result a measurement at the STS would be a natural follow-on since the increased moderator brightness and improved neutron guide technology are estimated to provide well over an order of magnitude more neutrons to the experiment. If this effort moves forward it would be funded by the DOE Office of Nuclear Physics, but it is included here since a port viewing the coldest, highest-flux moderator would be required.

Science Drivers

Measurements of electric dipole moments of fundamental particles are considered high-priority by the U.S. nuclear and particle physics community as evidenced in numerous national advisory committee recommendations over the past decade. This is due to the connection between time-reversal invariance violation (TRIV) manifest in a non-zero electric dipole moment in a fundamental particle and the currently unknown physical process responsible for the existence of matter in the universe.

Matter requires a small asymmetry between matter and anti-matter, otherwise all matter/anti-matter would have annihilated immediately following the big bang. Such an asymmetry requires physical processes outside the current standard model (SM) of particle physics. Extensions of the SM naturally include processes that lead to non-zero EDMs for neutrons. As a result, experiments to measure the neutron's electric dipole moment have been carried out essentially continuously for the past 65 years, with the current best precision corresponding to a separation of opposite charge centers in the neutron that is smaller than one trillionth the diameter of the neutron. Measurements to date have eliminated many theories. Most current theories predict neutron EDMs large enough to be observed by the measurement currently being mounted at the SNS. If that measurement reaches its statistical limit – no matter the result – there will be a strong scientific push to take advantage of the additional neutron intensity available at the STS.

Science Requirements

The nEDM@STS experiment will use a superthermal process to generate ultracold neutrons (UCN) (E < 200 nEV) from the scattering of 8.9Å neutrons by liquid helium. The experiment's statistical precision is inversely proportional to the square root of the number of neutrons, so the key scientific requirement is maximizing the fluence of 8.9Å neutrons. This requires a port on a cold coupled moderator large enough to fit an expanding neutron "horn" feeding a ballistic guide.

Preliminary neutron extraction calculations simulations suggest that the anticipated high average cold flux at the STS, coupled with an optimal ballistic guide, would provide well over an order of magnitude more UCN than will be available at the current SNS BL-13. Of course, if a very cold neutron source was incorporated at the STS, a significantly greater gain would be realized.

Tight control of the magnetic environment is key to any EDM experiment. Maximum allowed gradients are a few ppm/cm. Great care has gone into the experiment design, which includes active cancellation coils, a multi-layer room-temperature magnetic shield and an inner superconducting shield. But it is important to start with a magnetically clean environment. The current SNS magnetic stray field boundary conditions are sufficient.

The nEDM experiment is large, requiring a building footprint of ~4,000 square feet. Significant power and cooling water are required to supply a helium liquefaction plant and the large pump stacks associated with the experiment's two high-power dilution refrigerators.

Technical Description

What follows is a technical description of the nEDM experiment currently being mounted at the FTS. Moderate upgrades may be required, but – assuming statistical limitation is achieved – it is anticipated moving the existing experiment in its entirety to the STS.

At the heart of the nEDM experiment is a three-component fluid, consisting of spin polarized ultracold neutrons (100-10,000 cm^{-3}) and spin-polarized ^3He ($^3He/^4He \sim 10^{-10}$) in a bath of isotopically purified liquid ^4He. The Helium-3 acts as a spin analyzer and a co-magnetometer. This system is subjected to a small (~100 mG) extremely uniform magnetic field (B) and a strong (~75 kV/cm) electric field (E). The signature for a non-zero EDM is a change in the neutron precession frequency proportional to E when the relative direction of the E and B fields are changed.

The neutron guide must deliver the maximum flux of polarized cold neutrons to the apparatus. The key technical requirement is a guide system that can capture the maximum phase space of neutrons, within a few percent bandwidth centered on 8.9Å. As noted above this implies a ballistic guide that begins as close to the moderator face as possible and has as high an "m" as practicable. It is critical that shielding and shutter penetrations be sufficient large to accommodate such a guide. The ultracold neutrons are created by scattering polarized 8.9Å neutrons off phonons in the Helium. Equipment in an auxiliary cryostat delivers the polarized Helium-3 and removes it when the measurement is over. The three-component fluid is held inside a pair of measurement cells mounted between a set of electrodes, all of which is held inside a multi-layer magnet coil and shielding package.

The neutron precession frequency is obtained from the time-dependence of neutron/^3He capture events, which due to the spin-dependent cross section, have a sinusoidal dependence with a frequency equal to the difference between the neutron and ^3He precession frequencies. The capture events produce an optical signal that must be converted from EUV to visible wavelengths before transmission to an array of photon detectors.

APPENDIX 5. WORKSHOP PARTICIPANTS

Douglas Abernathy Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 abernathydl@ornl.gov	Haile Ambaye Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 ambayeh@ornl.gov
Ken Andersen European Spallation Source Tunavägen 24 223 63 Lund, Sweden Ken.andersen@esss.se	David Anderson Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 andersondc@ornl.gov
John Ankner Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 anknerjf@ornl.gov	David Arakawa DOE ORNL Site Office P.O. Box 2008 Oak Ridge, TN 37831 arakawadk@ornl.gov
Goran Arbanas Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 arbanasg@ornl.gov	Kevin Berry Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 berrykd@ornl.gov
Jonas Birk Paul Scherrer Institute 5232 Villigen PSI Switzerland jonasobirk@gmail.com	Annette Bodenheimer North Carolina State University 20 Watauga Club Drive Raleigh, NC 27695 AnnetteBodenheimer@gmail.com
Mark Bowden Pacific Northwest National Laboratory 902 Innovation Boulevard Richland, WA 99352 mark.bowden@pnnl.gov	Robert Briber University of Maryland 1109 Chemical and Nuclear Eng. Bldg. College Park, MD 20742 rbriber@umd.edu
Craig Bridges Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 bridgesca@ornl.gov	Collin Broholm Johns Hopkins University 3400 North Charles Street Baltimore, MD 21218 broholm@jhu.edu
Stuart Campbell Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 campbellsi@ornl.gov	Huibo Cao Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 caoh@ornl.gov
Bryan Chakoumakos Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 chakoumakobc@ornl.gov	Julian Chen Los Alamos National Laboratory P.O. Box 1663 Los Alamos, NM 87545 chen_j@lanl.gov

Yongqiang Cheng Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 chengy@ornl.gov	Songxue Chi Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 chis@ornl.gov
Andrew Christianson Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 christiansad@ornl.gov	Leighton Coates Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 coatesl@ornl.gov
Matthew Connolly National Institute of Standards and Technology 325 Broadway Boulder, CO 80305 matthew.connolly@nist.gov	David Cowburn Albert Einstein College of Medicine 1300 Morris Park Avenue Bronx, NY 10461 david.cowburn@einstein.yu.edu
Michael Crawford DuPont Company DuPont Experimental Station, E400/5424 Wilmington, DE 19803 michael.k.crawford@dupont.com	Lowell Crow Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 crowmljr@ornl.gov
Mark Dadmun University of Tennessee Buehler Hall 1420 Circle Drive Knoxville, TN 37996 dad@utk.edu	Luke Daemen Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 daemenll@ornl.gov
Pengcheng Dai Rice University 6100 Main Street Houston, TX 77005 pdai.utk@gmail.com	Lisa DeBeer-Schmitt Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 debeerschmlm@ornl.gov
Iain Dixon National High Magnetic Field Laboratory 1800 East Paul Dirac Drive Tallahassee, FL 32310 dixon@magnet.fsu.edu	Changwoo Do Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 doc1@ornl.gov
Michelle Dolgos Oregon State University 153 Gilbert Hall Corvallis, OR 97331 michelle.dolgos@oregonstate.edu	Takeshi Egami University of Tennessee P.O. Box 2008 Oak Ridge, TN 37831 egami@utk.edu
Georg Ehlers Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 ehlersg@ornl.gov	Morten Eskildsen University of Notre Dame 225 Nieuwland Science Hall Notre Dame, IN 46556 eskildsen@nd.edu
Barbara Evans Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 evansb@ornl.gov	Lawrence Falvello University of Zaragoza Pedro Cerbuna 12, Zaragoza Aragon 50009 falvello@unizar.es

Antonio Faraone NIST Center for Neutron Research 100 Bureau Drive Gaithersburg, MD 20899-6100 afaraone@nist.gov	Jaime Fernandez-Baca Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 fernandezbja@ornl.gov
Millicent Firestone Los Alamos National Laboratory P.O. Box 1663 Los Alamos, NM 87545 firestone@lanl.gov	Michael Fitzsimmons Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 fitzsimmonsm@ornl.gov
Emiliano Fratini University of Florence Piazza San Marco, 4 Florence, Tuscany 50121 emiliano.fratini@unifi.it	John Galambos Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 galambosjd@ornl.gov
Ovidiu Garlea Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 garleao@ornl.gov	Bruce Gaulin McMaster University 1280 Main Street W. Hamilton, Ontario L8S4M1 bruce.gaulin@gmail.com
Oksana Gerlits Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 gerlitsoo@ornl.gov	Chad Gillis Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 gillisrc@ornl.gov
Gnana Gnanakaran Los Alamos National Laboratory P.O. Box 1663 Los Alamos, NM 87545 gnana@lanl.gov	John Gordon Los Alamos National Laboratory P.O. Box 1663 Los Alamos, NM 87545 jgordon@lanl.gov
Richard Goyette Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 goyetterj@ornl.gov	Garrett Granroth Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 granrothge@ornl.gov
Geoffrey Greene University of Tennessee Neilsen Physics Bldg 401 Knoxville, TN 37996 ggreene@utk.edu	Sudipta Gupta Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 g.sudipta26@gmail.com
Masato Hagihara Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 hagiharam@ornl.gov	William Hamilton Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 hamiltonwa@ornl.gov
Youngkyu Han Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 hany@ornl.gov	Thomas Hansen Institut Laue-Langevin 71 avenue des Martyrs Grenoble, Rhone-Alpes 38000 hansen@ill.fr

Sara Haravifard Duke University 120 Science Dr., Dept of Physics Durham, NC 27708 haravifard@phy.duke.edu	William Heller Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 hellerwt@ornl.gov
Raphael Hermann Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 hermannrp@ornl.gov	Luke Heroux Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 herouxla@ornl.gov
Ken Herwig Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 herwigkw@ornl.gov	Rex Hjelm Los Alamos National Laboratory P.O. Box 1663 Los Alamos, NM 87545 hjelm@lanl.gov
Jason Hodges Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 hodgesj@ornl.gov	Kunlun Hong Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 hongkq@ornl.gov
Tao Hong Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 hongt@ornl.gov	Camden Hubbard Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 camden.hubbard@me.com
Thomas Huegle Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 hueglet@ornl.gov	Ashfia Huq Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 huqa@ornl.gov
Richard Ibberson Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 ibbersonrm@ornl.gov	Erik Iverson Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 iversoneb@ornl.gov
David Jacobson National Institute of Standards and Technology 100 Bureau Drive Stop 8461, Bldg. 235, Rm K133 Damascus, MD 20879-8461 david.jacobson@nist.gov	Marc Janoschek Los Alamos National Laboratory P.O. Box 1663 Los Alamos, NM 87545 mjanoschek@lanl.gov
Tae Hui Kang Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 kangt@ornl.gov	Yoon Kang Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 kangyw@ornl.gov
John Katsaras Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 katsarasj@ornl.gov	Maciej Kawecki Uppsala University Box 516 751 20 Uppsala, Sweden maciej.kawecki@physics.uu.se

Abebe Kebede North Carolina A&T State University 1601 East Market Street Greensboro, NC 27411 gutaye@ncat.edu	Boris Khaykovich Massachusetts Institute of Technology 77 Massachusetts Ave., NW13-242 Cambridge, MA 02139 bkh@mit.edu
Choel Kim Baylor College of Medicine Alkek N520.07, One Baylor Plaza Houston, TX 77030 ckim@bcm.edu	Young-June Kim University of Toronto 60 St. George Street Toronto, Ontario M5S 1A7 yjkim@physics.utoronto.ca
Alexander Kolesnikov Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 kolesnikovai@ornl.gov	Andrey Kovalevsky Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 kovalevskyay@ornl.gov
Ivan Kravchenko Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 kravchenkoii@ornl.gov	Joanna Krueger University of North Carolina, Charlotte 9201 University City Blvd. Charlotte, NC 28223 jkkruege@uncc.edu
Susan Krueger NIST Center for Neutron Research 100 Bureau Drive, Stop 6102 Gaithersburg, MD 20899-6102 susan.krueger@nist.gov	Tonya Kuhl University of California, Davis One Shields Ave., Dept. Chemical & Mat'l Science Davis, CA 95616 tlkuhl@ucdavis.edu
Stephen Kuhn University of Notre Dame P.O. Box 2008 Oak Ridge, TN 37831 skuhn2@nd.edu	Rajeev Kumar Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 kumarr@ornl.gov
Jyotsana Lal Louisiana State University Chemistry and Materials Science Baton Rouge, LA 70803 jlal@anl.gov	Paul Langan Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 langanpa@ornl.gov
John Larese University of Tennessee 552 Dabney-Buehler Hall, 1416 Circle Dr. Knoxville, TN 37996-1600 jzl@utk.edu	Ana Larralde University of Buenos Aires Viamonte 430/44, Buenos Aires, Buenos Aires Province C1053ABJ alarralde@qi.fcen.uba.ar
Hans Jochen Lauter hjlauter@gmail.com	Valeria Lauter Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 langanpa@ornl.gov
Nick Lavrik Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 lavriknv@ornl.gov	Chris Leighton University of Minnesota 151 Amundson Hall, 421 Washington Ave SE Minneapolis, MN 55455 leighton@umn.edu

Jonathan Leiner University of Notre Dame P.O. Box 2008 Oak Ridge, TN 37831 jleiner@alumni.nd.edu	Chen Li Carnegie Institute for Science 1530 P Street NW Washington, DC 20005 cli@carnegiescience.edu
Kuo Li Center for High Pressure Science and Technology Advanced Research 1690 Cailun Rd, Bldg 6, Pudong, Shanghai, 201203 likuo@hpstar.ac.cn	Ken Littrell Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 littrellkc@ornl.gov
Yaohua Liu Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 liuyh@ornl.gov	Yun Liu NIST/University of Delaware 100 Bureau Drive, MS6102 Gaithersburg, MD 20899 yunliu@nist.gov
Brad Lokitz Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 lokitzbs@ornl.gov	Mark Lumsden Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 lumsdenmd@ornl.gov
Dong Ma Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 dongma@gmail.com	Robin Macaluso University of Texas 700 Planetarium Place Arlington, TX 76019 robin.macaluso@uta.edu
Jaroslaw Majewski Los Alamos National Laboratory P.O. Box 1663 Los Alamos, NM 87545 jarek@lanl.gov	Charles Majkrzak NIST Center for Neutron Research 100 Bureau Drive, Stop 6102 Gaithersburg, MD 20899-6102 charles.majkrzak@nist.gov
Eugene Mamontov Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 mamontove@ornl.gov	Masaaki Matsuda Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 matsudam@ornl.gov
Steve May Drexel University 3141 Chestnut St., 344 LeBow Engineering Bldg. Philadelphia, PA 19104 smay@coe.drexel.edu	William McHargue Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 mcharguewm@ornl.gov
Tyrel McQueen Johns Hopkins University 3400 N. Charles St. Baltimore, MD 21218 mcqueen@jhu.edu	Rob McQueeney Iowa State University Dept. of Physics & Astronomy Ames, IA 50011 Rjmcqueeney@gmail.com

Flora Meilleur ORNL/North Carolina State University P.O. Box 2008 Oak Ridge, TN 37831 meilleurf@ornl.gov	Tommy Michaelides Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 michaelidesc@ornl.gov
Diana Mitrea St. Jude Children's Hospital 262 Danny Thomas Place, MS 311 Memphis, TN 38105 diana.mitrea@stjude.org	Adam Moule University of California, Davis Chemical Engineering, 1 Shields Ave. Davis, CA 95616 amoule@ucdavis.edu
Martin Mourigal Georgia Institute of Technology School of Physics, 837 State Street Atlanta, GA 30332 mourigal@gatech.edu	Stephen Nagler Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 naglerse@ornl.gov
James Neilson Colorado State University 1872 Campus Delivery Fort Collins, CO 80524 james.neilson@colostate.edu	Jennifer Niedziela Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 niedzielajl@ornl.gov
Brad O'Dell ORNL/North Carolina State University P.O. Box 2008 Oak Ridge, TN 37831 wbodell@ncsu.edu	Daniel Olds Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 oldsdp@ornl.gov
Ryan Oliver Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 oliverrc@ornl.gov	Bradley Olsen Massachusetts Institute of Technology 77 Massachusetts Ave., Room 66-558a Cambridge, MA 02139 bdolsen@mit.edu
Hugh O'Neill Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 oneillhm@ornl.gov	Raymond Osborn Argonne National Laboratory 9700 South Cass Avenue Lemont, IL 60439 rosborn@anl.gov
Naresh Osti Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 ostinc@ornl.gov	Katharine Page Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 pagekl@ornl.gov
John Parise Stony Brook University 238 Earth and Space Sciences B1 Stony Brook, NY 11794-2100 john.parise@stonybrook.edu	Andre Parizzi Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 parizziad@ornl.gov
Andrew Payzant Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 payzanta@ornl.gov	Dayakar Penumadu University of Tennessee 312 John D. Tickle Eng. Bldg; 851 Neyland Dr Knoxville, TN 37996-2313 dpenumad@utk.edu

Edmund Perfect University of Tennessee 210 Earth & Planetary Sciences Bldg, 1412 Circle Dr Knoxville, TN 37996-1410 eperfect@utk.edu	Josh Pierce Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 piercejj@ornl.gov
Philip Pincus University of California at Santa Barbara 3004A Materials Research Laboratory Santa Barbara, CA 93106-5050 fyl@mrl.ucsb.edu	Sai Venkatesh Pingali Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 pingalis@ornl.gov
Nayomi Plaza University of Wisconsin, Madison Materials Sci and Eng Bldg; 1509 University Ave Madison, WI 53706 nplaza@wisc.edu	Abhijit Pramanick City University of Hong Kong Tat Chee Avenue, Kowloon Tong Hong Kong abhijit.pramanick@gmail.com
Thomas Proffen Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 tproffen@ornl.gov	Marc Pusey iXpressGenes, Inc. 601 Genome Way Huntsville, AL 35806 marc.pusey@ixpressgenes.com
Roger Pynn Indiana University 2401 Milo B Sampson Lane Bloomington, IN 47408 rpynn@indiana.edu	Shuo Qian Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 qians@ornl.gov
Durgesh Rai Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 raidk@ornl.gov	Timmy Ramirez-Cuesta Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 ramirezcueaj@ornl.gov
Yang Ren Argonne National Laboratory 9700 S Cass Avenue Lemont, IL 60439 yren@anl.gov	Lee Robertson Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 robertsonjl@ornl.gov
Stephan Rosenkranz Argonne National Laboratory 9700 S Cass Avenue Lemont, IL 60439 srosenkranz@anl.gov	Anjana Samarakoon University of Virginia PO Bx 400714 Dept of Physics; 382 McCormick Rd Charlottesville, VA 22903 Ams4ux@virginia.edu
Luis Sanchez Diaz Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 sanchezdizal@ornl.gov	Andrei Savici Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 saviciat@ornl.gov

Crystal Schrof Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 schrofca@ornl.gov	Gerald Schneider Louisiana State University 331 Chemistry and Materials Bldg Baton Rouge, LA 70803 gjschneider@lsu.edu
Harley Skorpenske Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 skorpenskehd@ornl.gov	Greg Smith Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 smithgs1@ornl.gov
Elinor Spencer Virginia Tech Integrated Life Sciences Bldg., 1981 Kraft Drive Blacksburg, VA 24060 espence@vt.edu	Shelby Stavretis University of Tennessee Buehler Hall 1420 Circle Drive Knoxville, TN 37996-1600 sstavret@vols.utk.edu
Matthew Stone Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 stonemb@ornl.gov	Susan Taylor University of California, San Diego 9500 Gilman Drive #0654 La Jolla, CA 92093-0654 staylor@ucsd.edu
Alexander Thaler Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 thaleran@ornl.gov	Kristina Thiagarajan Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 thiagarajakd@ornl.gov
Wei Tian Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 tianwn@ornl.gov	Xin Tony Tong Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 tongx@ornl.gov
John Tranquada Brookhaven National Laboratory PO Box 5000; Bldg. 734 Upton, NY 11973-5000 jtran@bnl.gov	Volker Urban Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 urbanvs@ornl.gov
Bogdan Vacaliuc Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 vacaliucb@ornl.gov	Venu Vandavasi Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 vandavasiv@ornl.gov
Adam Vogt Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 vogtaj@ornl.gov	Jinchen Wang University of Kentucky 410 Administration Dr. Lexington, KY 40506 jinchenwang0401@gmail.com
Meng Wang University of California, Berkeley 311 Birge Hall Berkeley, CA 94720 wangm@berkeley.edu	Shanmin Wang Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 wangs@ornl.gov

Xiaoping Wang Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 wangx@ornl.gov	Hubertus Weijers Florida State University 600 W. College Ave., A0300 MAG Tallahassee, FL 32306 weijers@magnet.fsu.edu
Kevin Weiss Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 weisskl@ornl.gov	Mark Wendel Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 wendelmw@ornl.gov
Kenneth Weston Nucsafe, Inc. 601 Oak Ridge Turnpike Oak Ridge, TN 37830 kweston@nucsafe.com	Pamela Whitfield Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 whitfieldps@ornl.gov
Claire White Princeton University Dept Civil & Environ. Eng Princeton, NJ 08544 whitece@princeton.edu	Christoph Wildgruber Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 wildgrubercu@ornl.gov
Angus Wilkerson Georgia Institute of Technology 901 Atlantic Dr. Atlanta, GA 30332-0400 angus.wilkinson@chemistry.gatech.edu	Robert Williams Los Alamos National Laboratory P.O. Box 1663 Los Alamos, NM 87545 rfw@lanl.gov
Travis Williams Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 williamstj@ornl.gov	Barry Winn Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 winnbl@ornl.gov
David Worcester NIST Center for Neutron Research 100 Bureau Drive, Bldg 235, E112, Mailstop 6102 Gaithersburg, MD 20899-6102 worcesterd@missouri.edu	Zili Wu Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 wuz1@ornl.gov
Ziling Ben Xue University of Tennessee Department of Chemistry Knoxville, TN 37996-0001 xue@utk.edu	Ming Yi University of California, Berkeley 309 Birge Hall Berkeley, CA 94720 ymormy@gmail.com
Igor Zaliznyak Brookhaven National Laboratory Bldg 734 ISB, CMPMS Upton, NY 11777 zaliznyak@bnl.gov	Qiu Zhang Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 zhangq@ornl.gov
Yang Zhang University of Illinois, Urbana-Champaign 901 West Illinois Street Urbana, IL 61801 zhyang@illinois.edu	Zhe Zhang Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 zhangz2@ornl.gov

Jinkui Zhao Oak Ridge National Laboratory P.O. Box 2008 Oak Ridge, TN 37831 zhaoj@ornl.gov	Haiyan Zheng Center for High Pressure Science and Technology Advanced Research 1690 Cailun Rd, Bldg 6, Pudong, Shanghai, 201203 zhenghy@hpstar.ac.cn
Piotr Zolnierczuk Juelich Research Center P.O. Box 2008 Oak Ridge, TN 37831 zolnierczukp@ornl.gov	