1 New Instruments at SNS and HFIR

ORNL is now well positioned to realize opportunities to build new instruments at the remaining 5 open beam ports at the SNS First Target Station (FTS), and to reposition instruments and build new instruments at HFIR. Over the next 5-10 years, the coordinated construction of new instruments—along with further improvements to existing instruments—will continue to provide researchers with cutting-edge neutron scattering capabilities to advance science discovery and solve the most challenging technology problems. And as we look to the future, it is important to proceed with an integrated approach that optimizes placement of new instruments across the current ORNL sources and the proposed SNS Second Target Station (STS).

Over the past three years ORNL completed a series of rigorous internal and external reviews of existing neutron scattering instruments at SNS and HFIR. The purpose was to improve the overall performance and productivity of these instruments, to be more responsive to community needs and technological advances, and to identify opportunities for improving or establishing new instrument capabilities in strategic areas of science. ORNL established a mechanism (the Science Productivity Process) and a rolling budget to enable these goals. The Science Productivity Process has already provided new capabilities and the first series of planned triennial reviews of the instrument suites at SNS and HFIR has been completed. These instrument suite reviews assessed the breadth and impact of the science on the respective instruments and, as part of their charge, reviewers considered the needs for new capabilitites across each instrument suite. Table 1 summarizes recommendations for new instruments at SNS and HFIR from these reviews.

Table 1. New instruments recommended for the current ORNL neutron sources by the external instrument suite reviews.

Review	Date	New instrument recommendations[a]
Powder Diffraction	Aug. 3-4, 2016	1. DISCOVER 2. HiResPD
SANS/Reflectometry	Jan. 24-25, 2017	High-throughput SANS (kSANS)
Single Crystal Diffraction	Jun. 27-28, 2017	none
Imaging and Engineering Science	Jun. 27-28, 2017	1. VENUS 2. (Need for texture measurement capability identified - MICRON)
Inelastic Scattering (TAS/ToF)	Nov. 14-15, 2017	MANTA
Inelastic Scattering (Chemical Spectroscopy)	Nov. 14-15, 2017	BeFAST and Neutron Spin Echo at HFIR

[a] The priority given by the review committee is reflected in the numbered order.

The diversity of ORNL source charateristics provides an unprecedented opportunity to position instrument types and neutron scattering techniques at the best source. This document summarizes the strengths of the ORNL neutron sources including the STS in Section 1.1. New instrument concepts, following the recommendations of the external instrument suite reviews (Table 1), are summarized in Sections 1.2 and 1.3, while the Appendix provides more complete descriptions. Concept development is advanced for the SNS VENUS, DISCOVER, and HiResPD instruments and the HFIR MANTA instrument. The remaining instrument concepts represent early thinking on what could be achieved.

1.1 ORNL Three Source Strategy

ORNL is unique among leading centers for neutron scattering in operating a high-power research reactor and a high-power spallation source at the same laboratory. These two types of neutron sources have complementary strengths. Operated continuously at 85 MW, HFIR excels at producing the maximum number of neutrons, resulting in high time-average neutron brightness. SNS produces fewer total neutrons but does so in short time bursts or pulses that are separated in time resulting in high instantaneous brightness as illustrated in Figure 1. HFIR has 200x and 90x the average neutron brightness of the FTS decoupled, para-H_2 moderator, while the FTS peak brightness is 10x and 3x that of HFIR at neutron wavelengths of 1 Å and 5 Å respectively. The SNS FTS is optimized to produce narrow neutron pulses at a high repetition rate with an emphasis on using thermal neutrons to support high wavelength resolution measurements using time-of-flight (ToF) techniques. The SNS STS will be optimized to produce high peak brightness and broader pulses of cold neutrons at lower frequency complementing the strengths of HFIR and FTS. At 5 Å, the STS geometrically optimized, cold coupled para-H_2 moderator will have 27x the peak brightness of the corresponding FTS moderator and 116x higher peak brightness than the HFIR cold source. Neutron scattering instrumentation is typically optimized to take advantage of either peak or average source neutron brightness, affording ORNL the opportunity to match instrument types and neutron scattering methods to the facility source that will maximize their scientific impact. In combination, these three neutron sources will provide the U.S. research community with access to the cutting-edge neutron scattering capabilities required to address the challenging science questions of the next decades.

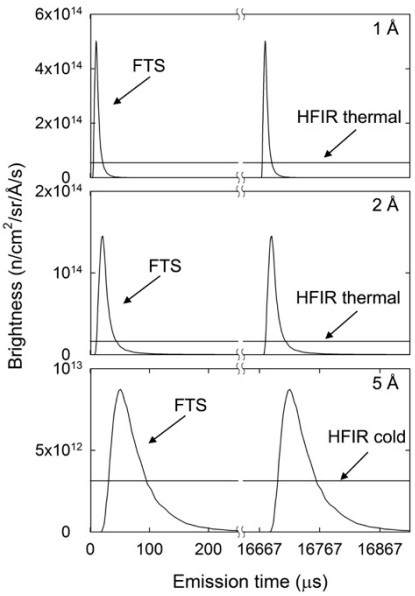

Figure 1. Pulsed neutron production at the SNS first target station operating at 1.4 MW and 60 Hz compared to the continuous neutron production of HFIR. Note the gap in the horizontal time axis.

Figure 2 compares the performance of HFIR and SNS in the context of current and future international sources. Reactors have the highest thermal and cold neutron average brightness of all current sources while short proton pulse sources have the highest peak brightness. (For short proton pulse spallation sources, the data shown are from the moderator that has the highest peak brightness unless another moderator is within 10% of this value and has a higher average brightness. As a consequence, the plots include a variety of moderator types.) The European Spallation Source (ESS), currently under construction, seeks to change this paradigm by operating in a long pulse mode at sufficient proton beam power to generate both high peak and high average brightness. When ESS reaches 5 MW of proton beam power it will have peak and average brightness comparable to the world's current best sources in the thermal neutron range and establish new thresholds for cold neutron production.

The SNS Proton Power Upgrade (PPU) project will double the accelerator power capability from 1.4 MW to 2.8 MW and provide the infrastructure to deliver 2 MW to FTS raising its thermal neutron performance to a leading level, especially for high wavelength resolution measurements that benefit from a high repetition rate. Construction of the STS will establish ORNL as the world leader in producing cold

neutron beams with highest peak brightness. Although STS will be optimized for the production of cold neutrons, its moderators will simultaneously produce bright pulses of thermal neutrons, although broader and at a lower repetition rate than FTS. HFIR will continue to provide the highest average thermal brightness and will be second only to a 5 MW ESS in delivering highest average cold neutron brightness.

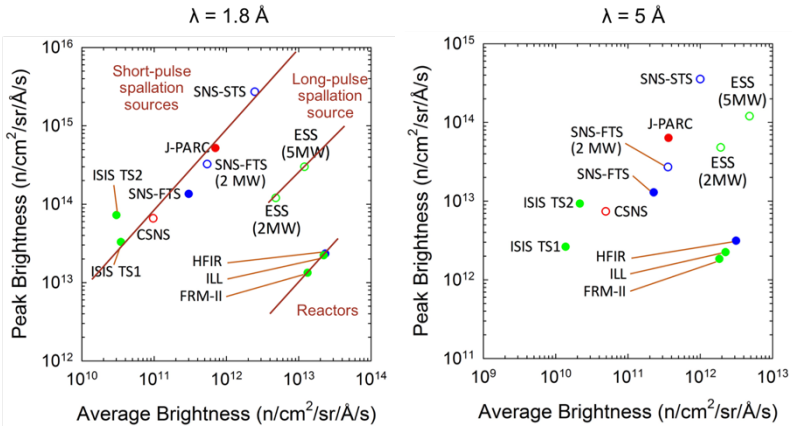

Figure 2. Comparison of average and peak neutron brightness of ORNL and international neutron sources. Left and right plots are for thermal and cold neutrons respectively. Closed circles are existing facilities while open circles represent planned upgrades and new facilities.

1.2 Future SNS Instruments

The five empty beam lines indicated in Figure 3 represent a significant opportunity to build next-generation neutron scattering instruments with new capabilities to address emerging science challenges. The characteristics of the moderators illuminating these beam lines are listed in Table 2. Apart from the moderator illuminating beam line 14A, they are all poisoned, decoupled moderators that are optimized to provide the high neutron wavelength resolution that is the strength of the FTS. The instrument concepts which have been developed are all located on these high-resolution beam lines.

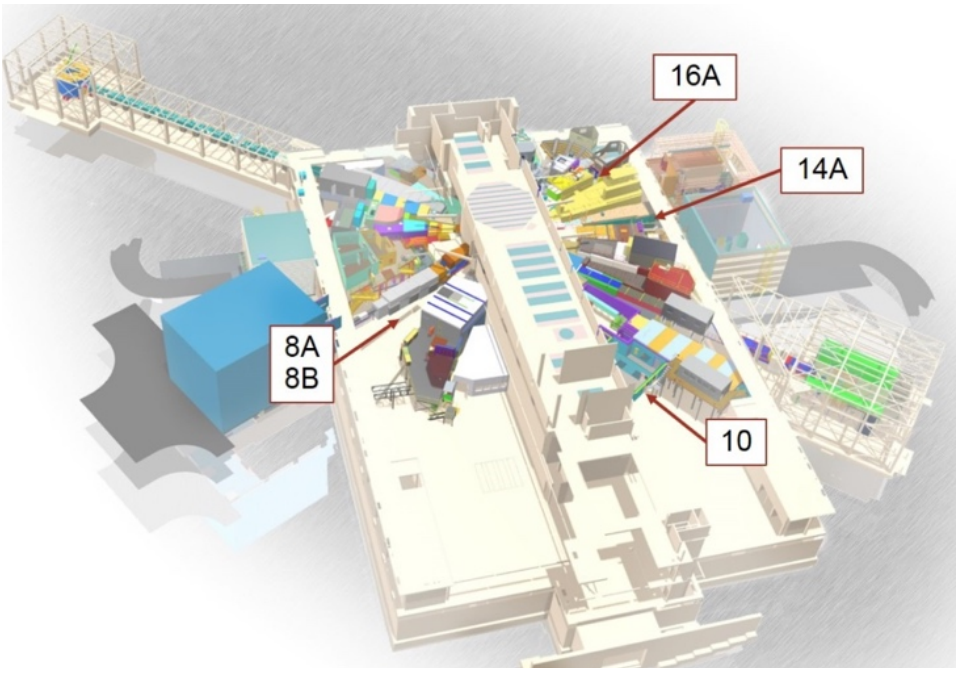

Figure. 3. SNS instrument layout showing empty beam lines.

Table 2. Description of the five empty beam lines at the SNS target station.

Beam Line	Moderator Type	Moderator Spectral Characteristics	Neighboring Instrument Types[a]
8A	Shallow-poisoned, decoupled, ambient H_2O	Sharp pulses of thermal neutrons; high λ-resolution	Diffractometer
8B	Shallow-poisoned, decoupled, ambient H_2O	Sharp pulses of thermal neutrons; high λ-resolution	Diffractometer
10	Poisoned, decoupled cold para-H_2	Sharp pulses of cold neutrons; high λ-resolution	Diffractometer
14A	Coupled, cold para-H_2	Broad pulses of cold neutrons; high flux	Cold neutron spectrometer
16A	Deep-poisoned, ambient H_2O	Broad pulses of thermal neutrons; high flux	Thermal neutron spectrometer

[a]The neighboring instrument type is provided to illustrate the current use of that moderator.

Table 3 lists instrument concepts that have been developed for SNS. VENUS and DISCOVER have been the subject of many workshops and extensive discussions with the user community and have been recommended for priority construction by several review and advisory committees. The HiResPD instrument concept was originally developed as a candidate for the STS but requires a high wavelength resolution moderator which has resulted in its re-assignment to a FTS on a to-be-decided beam line at FTS that will support an ≈100 m long instrument. The remaining instrument concepts are at an earlier stage of development.

Table 3. New instrument concepts considered for SNS.

Instrument	Beam line	Technique	Description	Science Areas
MICRON	8A	Diffraction	Diffractometer to measure microstructure (texture) and phase transformation	Materials Engineering, geology
DISCOVER	8B	Diffraction	Diffractometer for materials discovery with simultaneous measurement of average and local structure able to follow the evolution of order in minutes	Chemistry, materials science, synthesis science
VENUS	10	Imaging	Wavelength-resolved TOF imaging supporting Bragg-edge and resonance imaging	Materials science, nuclear energy, electrical energy storage, geosciences, industry
BeFAST	16A	Spectroscopy	Inverse geometry spectrometer optimized for high energy transfers from 3000 cm^{-1} to 8000 cm^{-1}	Catalysis and "real-world" systems
HiResPD	TBD	Diffraction	High-resolution powder diffractometer for accurate sturucture factor determination of complex structures able to detect slight symmetry breaking	Materials science

MICRON – MICRON (Measurement of In-situ CRystallographic Orientation) is a compact, high flux neutron diffractometer with the focus of exploring a material's crystallographic orientation distribution or texture under extreme conditions. It is envisaged as a relatively short beam line with its sample position 18 m from the moderator located at beam line 18A viewing the high-resolution water moderator. Its 3.5Å bandwidth and high resolution 3x3 mm^2 pixel size 2D scintillator detectors provides a Q range coverage from 1$Å^{-1}$ to 24$Å^{-1}$ and enabling acquisition of full pole figures with minimum sample rotation. Open access to the sample position is illustrated in Figure 4 will enable a wide range of sample environments. Texture and phase transformations can be measured in situ or in operando with extreme external stimuli, such as temperature, pressure, and electrical fields, etc. MICRON will fill the capability gap in texture measurement left when the Lujan HIPPO instrument became unavailable to general users and will also open new fundamental and applied science opportunities for academia as well as industry. Initial performance estimates are that the instrument will have approximately 10x higher neutron flux at the sample position relative to HIPPO.

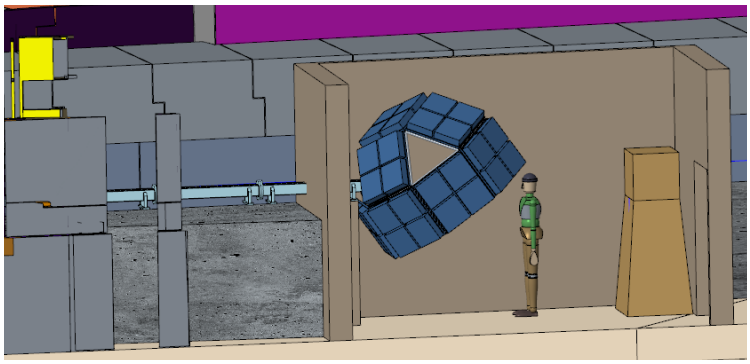

Figure 4. Schematic view of the sample area for MICRON.

DISCOVER – DISCOVER combines the advantages of high-Q resolution and wide Q-range ToF neutron scattering with low and stable background to study real materials in their operating environments. It will complement the high-flux, wide-Q diffraction/total scattering instrument NOMAD and the medium-high resolution POWGEN diffractometer. Day one capabilities include simultaneous measurement of average (diffraction) and local (PDF) structure and ability to follow the evolution of order on a time scale of minutes. The instrument will be located on beam line 8B and leverage the high-wavelength resolution side of the SNS water moderator. Figure 5 shows a schematic view of the instrument.

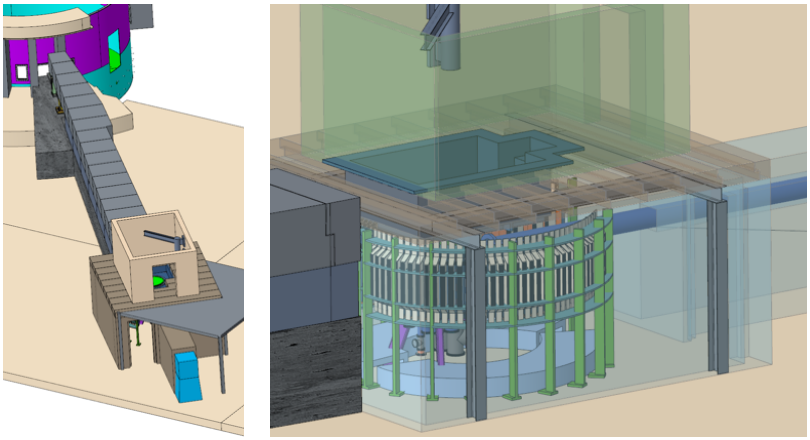

Figure 5. Schematic view of DISCOVER at beam line 8B. The left figure illustrates the beam line layout while the image on the right illustrates the sample/detector area.

VENUS – VENUS is a wavelength-resolved, time-of-flight, neutron imaging station seeking to bridge measurements across multiple length and time scales to understand, predict and control properties of novel functional materials. The instrument will be optimized for the measurement of microscale structures using both radiography and computed tomography providing academia, industry, and government laboratories with the opportunity to advance scientific research in advanced manufacturing methods such as additive manufacturing, energy, materials, transportation, engineering, industrial technologies, geosciences, plant physiology, and biology. Its Day 1 capbilities will include real-time simultaneous attenuation-based imaging and microstructure imaging (Bragg-edge) to study materials in situ and in operando and elemental (isotopic) imaging using adsorption resonances and prompt gamma methods. Figure 6 shows the VENUS concept located on beam line 10 with a 25 m moderator-sample distance providing high wavelength resolution, $\Delta\lambda/\lambda \leq 0.15\%$.

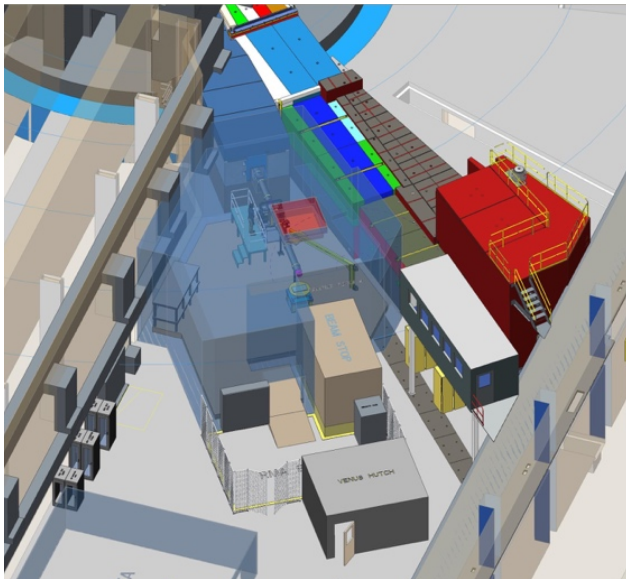

Figure 6. Schematic view of VENUS located on beam line 10 at the SNS.

BeFAST – BeFAST is a filter spectrometer that would complement VISION (BL-16B) by extending the useful range of energy transfers to 8000 cm^{-1} overlapping the range typically measured by Raman and Infrared spectroscopy. This energy range is particularly important in catalysis in the identification of C-H bonds and O-H stretches. This extended energy range will also enable extraction of reliable anharmonic parameters important for computational chemistry without the selection rules that limit the usefulness of Raman and Fourier transform infrared spectroscopy. As an instrument optimized to measure these large energy transfers, initial estimates indicate that BeFAST will have approximately 5000x higher count rates than VISION for energy transfers greater than 2000 cm^{-1}, capable of measurments as fast as 10 min for 0.5 gm hydrogenous samples. Figure 7 compares calculated spectra for VISION and BeFAST showing the complementarity of the two instruments. The instrument would be compact and take advantage of the high thermal brightness and resolution of the SNS poisoned moderator. With its emphasis on short neutron wavelengths, the instrument requires a very simple (no guide) optics system. Final energy resolution is provided by a beryllium filter and energy transfer resolution would be approximately 2% over the range of interest.

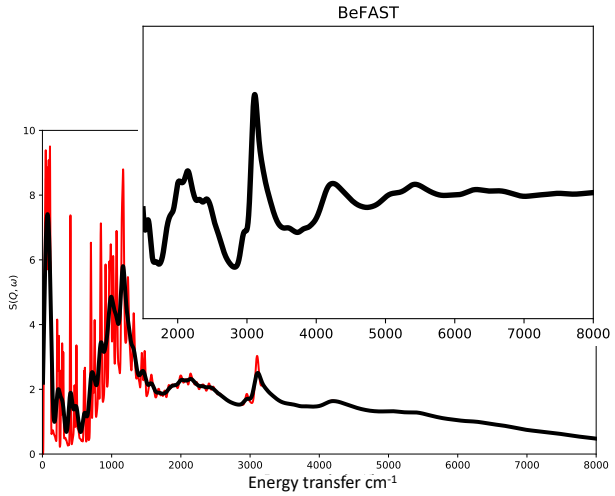

Figure 7. Neutron inelastic spectra calculated for triphenylmethane for VISION (red) and BeFAST (black).

HiResPD – HiResPD is a high-resolution powder diffractometer complementing the existing and planned suite of diffraction instruments at the SNS first target station with Δd/d as low as 0.024% in backscattering (2θ=170 deg) at lowest beam divergence of 1.22 mrad (0.032% at 7.35 mrad). The instrument would provide accurate structure factor determination of complex systems, detect slight symmetry breaking emerging from weak interactions on temperature and field, and coupled with advances in algorithm development and computing power, take steps towards ab initio structure determination from neutron powder data. An innovative design of the adaptive neutron optics package provides the capability to tune the neutron beam divergence from 1.2 to 10 mrad. The instrument requires a decoupled, poisoned high wavelength-resolution para-hydrogen moderator as used for POWGEN, and one able to support a 100 m long flight path from the moderator to the sample to provide the required wavelength resolution. Figure 8 is a schematic view of the detector and sample arrangement.

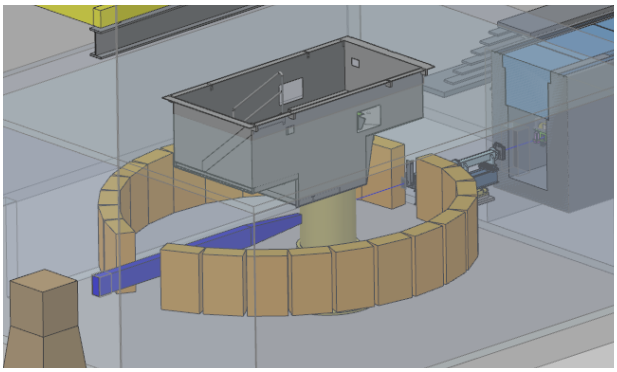

Figure 8. Schematic view of the sample and detector area for HiResPD.

1.3 Future HFIR Instruments

The upcoming HFIR outage to replace the permanent beryllium reflector represents an opportunity to re-optimize the HFIR cold guide hall. Minor modifications to the beam tube housing the horizontal cold source and the main shutter will allow closer placement of neutron guide to the cold source. Moving 1 m closer will facilitate about a 50% gain in neutron phase space that can be collected by the guide system enabling more end stations in the HFIR cold guide hall. Figure 9 shows a possible split of the guides at the start of the common casing just downstream of the main shutter. This new concept will maximize use of the HFIR cold source, increase utilization of the beam lines, improve performance of existing instruments, and allow for new instrument end stations as discussed below.

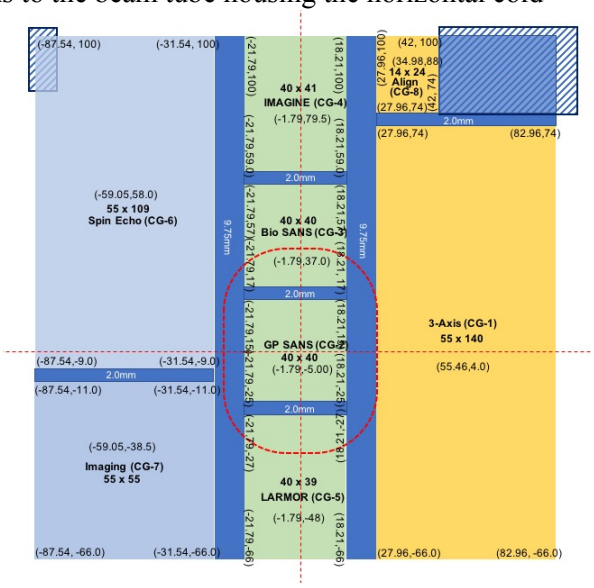

Figure 9. Possible guide division at entrance to the common casing (4.66m from the cold source). Cross-hatched regions are shadowed by up-stream hardware. The area labeled Spin Echo could alternatively be used to illuminate kSANS.

Table 4 lists instrument concepts that have been developed for the HFIR cold guide hall. MANTA and NSE at HFIR have been the topic of several workshops with the science community and their input is being incorporated into the instrument concepts. The kinetic SANS (kSANS) is at an earlier stage of development.

Table 4. New instruments under consideration for the HFIR guide hall.

Instrument	Beam line	Technique	Description	Science areas
MANTA	CG-1	Cold neutron spectroscopy	Cold neutron spectrometer with multiplexed analyzer array	Quantum materials, magnetism
kSANS	CG-X	SANS	High flux, high dynamic range SANS optimized for kinetic studies	Complex soft matter, proteins, polymers, synthesis science
NSE at HFIR	CG-X	NSE spectroscopy	High-resolution, NSE instrument reaching long Fourier times	Soft matter, biology/biophysics, quantum and magnetic materials

MANTA — MANTA is a state-of-the-art cold neutron spectrometer concept proposed for the CG-1 cold neutron guide. It would be a versatile, high-intensity instrument providing excellent energy and wave vector resolution in the cold neutron range and would replace the CTAX currently at CG-4C. The design will incorporate the most recent advances in neutron optics, which—combined with the high brightness of the HFIR cold source—will result in one of the most intense monochromatic beams in the world, enabling inelastic scattering studies on small samples (a few mm^3). The instrument would use a crystal monochromator and focusing optics to provide high incident neutron flux (>100× more than the current CTAX instrument). The existing CTAX analyzer would be complemented by a modern multiplexing analyzer that enables simultaneous measurements over a wide range of scattering angles and multiple final energies as shown in Figure 10. This would allow rapid mapping of excitations in the scattering plane while preserving the ability to measure with high flux in a localized region of Q,ω space, as required for parametric studies. It would also be designed with full neutron polarization capabilities, allowing for polarization-dependent measurements of S(Q,ω), and a resonant-spin-echo option leveraging the recent development of Wollaston prisms for ultra-high energy resolution.

Figure 10. Schematic view of MANTA with single analyzer (left) and multiplex analyzer (right).

kSANS – kSANS is a high flux, high dynamic range SANS instrument optimized for kinetic studies. With plans to operate from the continuous cold source at HFIR, kSANS will be equipped with a velocity selector and chopper system to allow both monochromatic and ToF modes of operation. The versatility afforded by this scheme for a SANS instrument will open many new scientific opportunities with particular advantages for performing new and challenging kinetic measurements. The vision is that kSANS will enable high-impact experiments, especially in biology and soft matter, where a high neutron flux coupled with enhanced time resolution will be most beneficial. This concept is at a very early stage of development. It is unlikely that both a kSANS and neutron spin echo could both be built given limitations on available neutron phase space and the geography of the guide hall. The performance of the instrument is compared with other SANS instruments in Figure 11.

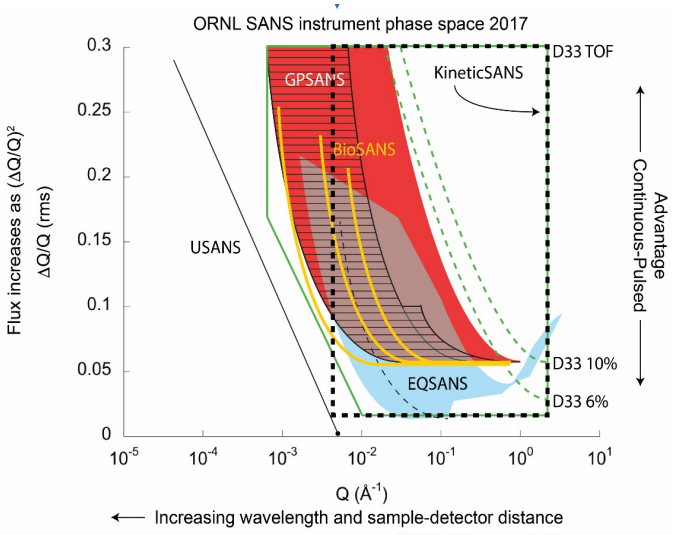

Figure 11. Phase space covered by the proposed kSANS in comparison with other SANS instruments.

NSE at HFIR — NSE at HFIR will be a new, IN-15 type, high-resolution spin echo spectrometer optimized for long wavelength neutrons, λ~8 Å and greater, to enable the best energy resolution that known technology can achieve. A high-level goal is to reach a correlation time of ~500 ns which will require λ~18 Å wavelength. The beam will be designed such that it will be converging on a relatively small cross section at the sample position, ~1-2 cm^2 area, which will enable studies of smaller samples. This will address the needs of the biological and medical communities by allowing the investigation of important biomolecules for drug research and drug delivery, that can be purified and deuterated in small quantities only, as well as to other research area of soft condensed matter like organic photovoltaics, biomimetic materials and polymeric membranes. This design feature will also be beneficial for studying the slow correlations in hard matter and new quantum materials.

2 Appendix A. Instrument Vignettes

The following are more complete write-ups of the instruments under consideration.

2.1 SNS BL-8A – MICRON, Measurement of In-situ CRystallographic Orientation by Neutrons

Abstract

MICRON will be a cost effective and compact high flux neutron diffractometer with the focus of exploring materials' crystallographic orientation distribution or texture under extremes. As one of the shortest SNS beamlines at about 18m, viewing the high-resolution water moderator at the port 8A and by using the available high flux neutron spectrum from FTS with 60 Hz chopper operation, MICRON has the potential to deliver one order of magnitude more neutron flux at its sample position as compared to the previous most advanced dedicated texture instrument in the U.S. Its 3.5Å bandwidth and high spatial resolution 3x3 mm^2 pixel size 2D scintillator detectors will provide Q-range coverage from $1Å^{-1}$ to $24Å^{-1}$ enabling acquisition of full pole figures with minimum sample rotations. The open access from the instrument's tail end will admit complex sample environments and a robotic sample changer to make MICRON one of the high throughput and versatile instruments at the FTS. Texture and phase transformation in wide varieties of materials can be measured in situ or in operando with extreme external stimuli, such as temperature, pressure, and electrical fields, etc. MICRON will not only restore general user access to the texture measurement capability that had been available at the Lujan Neutron Scattering Center HIPPO instrument but will also open new fundamental and applied science opportunities for academia as well as industry.

Science Case

Texture (the distribution of crystallographic orientations of a polycrystalline sample) is a fundamental material property seen in many natural systems and almost all engineered materials. Examples include composites (e.g., crystalline inclusions in a matrix); manufactured alloys for mechanical components (e.g., rolled metals); natural minerals; and polycrystalline and epitaxial multilayered structures (e.g., thin films, laminates, coatings, magnetic heterostructures). The analysis of texture and related changes in microstructure is critical for understanding and controlling many anisotropic materials properties, including mechanical integrity, chemical reactivity, electron conductivity, ion intercalation pathways, radiation damage resistance, magnetic susceptibility, and structural or functional failure mechanisms. Texture modifies the intensities of measured diffraction peaks, and this effect can be accurately modeled in different ways. Unaccounted texture will correlate with site occupancies and quantitative phase analysis of multiphase samples unpredictably and will lead to gross errors. The ability to accurately determine texture is prerequisite to developing the understanding necessary to control preferred orientation with the goal to improve physical properties mentioned above. MICRON will be a key enabling instrument for the texture sciences by taking advantage of its advanced detector technology with optimized discrete coverage, versatile sample environments, and the high flux of neutrons at the FTS. MICRON will uniquely enable detailed investigation of dynamic processes or spontaneous material responses, such as phase evolution and symmetry changes, crystallization, and texture evolution. Texture and grain movement, formation, and progression can be followed in situ with applied external conditions like temperature, pressure, magnetic, and/or electric fields, leading to thorough understanding of material properties optimization during materials processing. The high flux will allow small or even thin samples which often possess strong texture correlated materials properties to be investigated in situ by MICRON.

MICRON is going to be a unique tool to investigate microstructure and phase transformation of materials for structure-properties relationship by taking advantages of high flux and high-resolution neutrons at FTS. Example science cases include:

- Understanding of structural materials anisotropic properties due to preferred grain orientation and phase transformation of critical engineering materials and composites, such as lightweight materials, and superalloys during advanced materials processing or fabrication.

- Kinetic evolution of microstructure and phase fraction of advanced materials during solidifications process, such as casting of high entropy alloys and laser additive manufacturing of metal structures.

- Twinning or domain dynamics of functional materials under external stimuli, such as (magnetic) shape memory alloys and ferroelectrics.

Technical Description

MICRON will reside at BL-8A at the FTS of SNS at 18 m from the high-resolution shallow-poisoned, decoupled ambient H_2O moderator as seen in Figure 1. It will deliver high flux and medium resolution by benefiting from the sharp neutron pulses produced by the thermal moderator. Figure 2 shows the neutron brilliance of MICRON at SNS compared to HIPPO at the Lujan Neutron Scattering Center. According to this estimation, the neutron flux at the MICRON sample position should be one order of magnitude higher than HIPPO. A typical sample size will be from a few cubic millimeters up to 125 mm^3, with a potential acceptance of thin film below millimeter thickness. As shown in the conceptual design of the instrument, a total of 28 2D 384x384 mm^2 scintillation area detectors with 3x3 mm^2 pixel size will be placed inside a sphere of 1 m radius from the sample position. Each detector covers 22.5 ^{o} by 22.5^o solid angle, and the layout is optimized for texture measurement with minimum sample rotation overlapping counts. The detectors are assembled in 7 banks of 4 detectors each, with their centers located at 2θ scattering angles of 144.7^o, 125.2^o, 90^o, 50.5^o, with two banks for each of the first three values and only one for the last. Tunable beam divergence will provide resolutions from 0.38% to 1.8% in Δd/d from different locations of the detectors. Eliminating low angle detector coverage allows access to the instrument sample position from MICRON's tail end with a wide entrance. Thus, a commercial robotic arm sample changer and a range of complex sample environments with one or more fields (furnace, pressure cell, cryo-magnet etc.) can be exchanged easily and conveniently to enable versatile operation. MICRON will be equipped with sample stage with XYZΩ supports and 1 T of weight capacity and allow mounting the various sample environments or small goniometers. MICRON is a cost effective and easy-to-be-built instrument, and it will benefit from available technologies for its detector and sample environments.

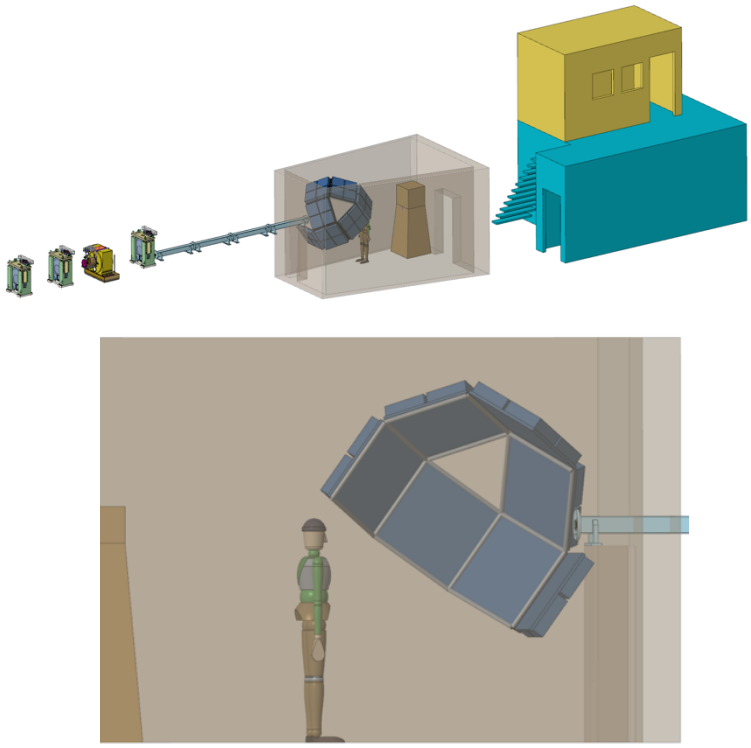

Figure 1. The conceptual design of MICRON at beam line 8A of FTS.

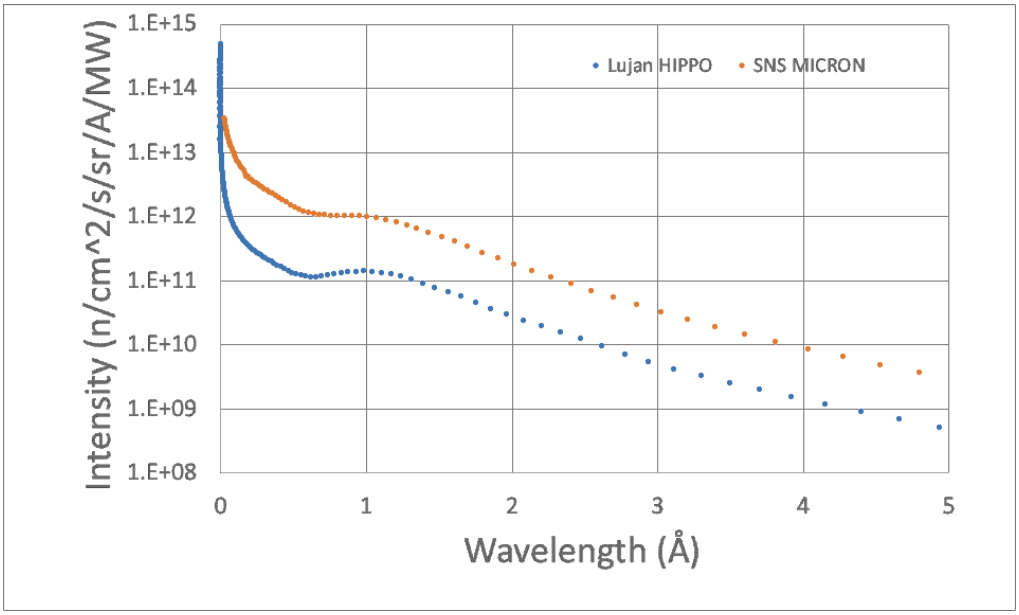

Figure 2. The neutron brilliance comparison of MICRON at SNS and HIPPO at the Lujan Neutron Scattering center.

Table 1. Key parameters of MICRON.

Parameter	Description
Moderator or Beam Line	High Resolution Water, SNS BL-8A
Beam Size at Sample	0.5 x 0.5 cm^2
Sample Size	Up to 0.5x0.5x0.5 cm^3
Moderator-sample distance	18 m
Sample-detector distance	1 m
Wavelength Range	0.2 Å $\leq \lambda \leq$ 5 Å
Q-range	$1Å^{-1} \leq Q \leq 24Å^{-1}$
Resolution	$\Delta d/d$ = 0.38~1.8%
Detector	384x384 mm^2 scintillator detectors with 3x3 mm^2 pixel size, and 7 banks of 4 detectors each to cover 33% of the sphere.

2.2 SNS BL-8B – DISCOVER, A Diffractometer for Materials Discovery

Abstract

The discovery of new materials has played an enabling role in all aspects of modern civilization, ushering in new energy, security, health, and information technologies. Many modern materials classes, from semiconductors and superconductors, to relaxor ferrolelectrics and ionic conductors, are defined by self-organization of atoms, spins, or charges occuring on length scales requiring understanding of both atomic and intermediate (several hundred Ångstrom) range order. There are a multitude of theories for such phenomena, but little in the way of experimental verification. For several years the Materials Chemistry and Quantum Condensed Matter communities have advocated for a rapid acquisition but medium-resolution and low background diffractometer for the First Target Station (FTS) at the Spallation Neutron Source (SNS), Oak Ridge National Laboratory (ORNL). DISCOVER, ORNL's Diffraction and Total Scattering Beamline for Materials Discovery, will be optimized for studying real materials in their operating environments from day one, and is intended to supply the scientific community with a platform for front-line investigations of the delicate interplay of global symmetry and local symmetry, for examining how order evolves from the atomic to macroscale, and for discovering how these features respond to external perturbation to deliver new functionality. Key scientific opportunities include:

- Developing fundamental and predictive understanding of reaction pathways and mechanisms, expanding the possible materials and structures that can be made.
- Developing a deep knowledge base of structure-property relationships for gas-solid interactions with sorbents and catalysts, advancing enhanced materials classes for chemical separations, conversion, and utilization.
- Observing and characterizing the structure, size, and responses of atom, spin, and charge correlations underpinning quantum material phenomena, ushering in new paradigms for controlling emergent states of matter.

The science case, early experiment opportunities, and key design criteria for the DISCOVER beamline concept are presented below.

Science Case

One of the transformative opportunities put forth in the 2015 Department of Energy Report *Challenges at the Frontiers of Matter and Energy* is "Understanding the critical roles of heterogeneity, interfaces, and disorder" in materials, underpinning the broader scientific priority to develop new approaches to control matter and realize new materials. DISCOVER answers the assertion that atomic and intermediate range order (and heterogeneity) need to be understood simultaneously and as they evolve to enable materials discovery and design. As such, DISCOVER will fill critical capability gaps for the exploration of synthesis science, quantum materials, and catalysis and sorption processes, to name a few. Several day-one opportunities are described below.

Reaction Pathways and Mechanisms. The reaction pathways by which solid-state materials form are typically unknown and multifaceted in their dependence upon experimental variables (e.g. temperature, pressure, chemical composition). The 2016 Basic Research Needs Report (BRN) *Synthesis Science for Energy Relevant Technologies* highlights that while broad longstanding emphasis on materials discovery and more recently, computational design has been in place, little effort has been directed to determine how materials form *during* reactions, impeding progress in materials synthesis and processing. Intermediates also play a seminal role, ultimately dictating final phase formation. These phases are often quenched out of final products, and therefore must be studied *in situ.* Neutrons are central to this

opportunity, due to abilities to penetrate reaction vessels and other sample environments, non-destructive interactions with matter, and especially sensitivity to light elements ubiquitous in synthesis science (such as H, Li, O, F, and S). **DISCOVER will enable quantitative insights into reaction pathways and mechanisms, as well as the presence and role of intermediate phases, defects, and non-idealities in the formation of new inorganic materials, including new ordered hierarchical and hybrid structures**. For example, there is a burgeoning landscape of metastable materials which cannot be accessed via conventional high temperature routes yet can be prepared via the careful transformation of pre-ordered amorphous or crystalline precursor phases. Such *topotactic conversion* takes place through selective atomic removal, insertion, or exchange reactions of a parent phase. Acid-loaded zeolites used in catalysis, olivine-structured NaMPO$_4$ (M=Fe, Mn) compounds used as Na-ion battery cathodes, superconducting Na$_x$CoO$_2$.nH$_2$O, and 2D MXenes materials are all modern material classes made this way, mostly with trial-and-error methods to date. DISCOVER will provide detailed mechanistic insight into structural rearrangements during reaction pathways with simultaneous diffraction (for crystalline phases) and high-fidelity PDF (for liquid, amorphous, and nanostructured/disordered phases), also providing the nature and chronology of any intermediate-range structural order as phases form. These capabilities will broadly apply to the preparation of hydrothermally prepared inorganic-organic hybrids, the flux growth of oxide-based compounds, and sol-gel techniques, to name a few.

Sorbent and Catalyst Performance. Catalysts and sorbents contribute over one trillion dollars to the national gross domestic product, yet specifics of adsorbate and chemically reactive environments remain almost entirely out of reach by traditional structural probes due to their aperiodic and transient nature. There is urgent need for capabilities to "visualize" adsorption of organic molecules in micropores and on surfaces, and at the same time, understand impacts to underlying structures, including their response and stability upon adsorption, desorption, uptake of water and other poisoning agents, lifetime cycling, and regeneration processes. Vast molecular dynamics efforts exist in these fields, requiring access to robust crystallographic and local structure information for validation. Neutron scattering offers light atom sensitivity, penetration of sample environment for *in situ/operando* analysis, and nondestructive analysis suitable for beam sensitive samples (e.g., zeolites) in this arena. The community is just now focusing on neutron studies with specific canonical examples. This opens key opportunity space for the DISCOVER beamline, where local correlations and their length-scales will be captured in real space with the PDF method and connected to long-range crystallographic information collected though high-resolution reciprocal space methods. **DISOVER will offer a holistic and fundamental understanding of the evolution and transformation of sorbents and catalysts *in operando*, leading to discovery of enabling structures, mechanisms, and ultimately new material designs.** A few specific questions to explore include: *How does water interact with carbide, carbon supported and coked catalyst surfaces, impacting performance? What roles do internal/external defects, dopants, and morphology play in the performance of catalysts for acid gas streams?* And *what chemistries, porosities, and defects enable self-healing and regeneration under real working conditions?* Other research aims will include the identity and mechanisms of small metal/oxide clusters in zeolite and other long-range ordered hosts, the short- to intermediate-range ordering in bimetallic catalysts (especially for metals with little atom difference such as Cu/Zn and Ni/Co), and unique hydrogen interaction issues (e.g., hydride formation in various metal and bimetallic catalysts).

Quantum Materials. The 2016 *Basic Research Needs Workshop Report on Quantum Materials for Energy Relevant Technologies* defines incredible opportunity space for controlling static or dynamic atomic, magnetic, or electronic states capable of responding to external perturbation to deliver new functionality. Many critical mesoscale features underpinning quantum materials emerge on 10 nm length scales difficult to access with existing powder instruments: ordering of Jahn-Teller polarons in manganites and colossal magnetoresistance, phase transition from high symmetry to low symmetry in martensitic phase transitions, and the impact of charge density wave fluctuations in layered superconductors, to name a few. As a theme, one seeks to understand how systems with extensively

degenerate ground states evolve into ordered states. Local symmetry is broken (e.g., decoration of dimers on a honeycomb lattice), but there is no long-range ordering of the motif. In the case of quantum magnets, there are a multitude of proposals for ordering on the mesoscale, with indirect evidence coming from observed excitation spectra, but direct insight into the structure and nature of these mesoscale orderings lacks concrete, experimental verification. In 10 years we not only want to be able to observe and characterize these entities, but also be able to control them, their structure, size, and responses. **DISCOVER will offer new opportunities to observe and characterize the structure, size, and response of atom, spin, and charge correlations underpinning quantum material phenomena, ushering in new paradigms for controlling emergent states of matter.** A tightly integrated sample environment suite coupling these capabilities to temperature, pressure, electronic and magnetic fields on day one will position the community to explore, for example, *Are nematic electronic states distinct from underlying mesoscale orthorhombicity in the iron high-temperature superconductors? What is the connection between observed inversion symmetry breaking and monoclinic symmetry in the electronic state, and the mesoscale atomic and magnetic structure of the high-Tc cuprates?* And *What is the mesoscale ground state selected to break degeneracy in geometrically frustrated quantum magnets?* In many cases, theoretical models are waiting for the structural data measured at the scales needed for validation.

Overarching Themes. As a common tenet, the above examples require detailed knowledge of long-range crystallographic order as well as quantification of the atomic local structure of materials, including defects, non-stoichiometries, and local chemical ordering. In each, recent and emerging breakthroughs in computational methods are providing a multitude of theories, while experimental validation remains sparse or incomplete. **Broadly, DISCOVER will explore the connection between global symmetry (i.e. that found over long lengthscales) and local symmetry (i.e. that found at the atomic scale), allowing us to explore how order evolves from the atomic to the macroscale.** A second critical capability will more directly enable quantification of the atomic structure of hydrogen and hydrogen bearing systems and species through use of a correlation chopper that separates out parasitic inelastic scattering contributions to neutron diffraction and neutron PDF signals. This will allow new opportunities to study materials as they are made and used, directly, without need of costly and time intensive synthesis and scale-up with specific isotopes. This capability may also separate static from dynamic contributions to diffraction signals in material structures, an area currently in proof-of-concept development.

Community Support. There is a rich history of community support for the DISCOVER beamline concept. At the user workshop "Delivering on the Promise of Powder Diffraction" in June 2013 at Oak Ridge National Laboratory, the scientific community proposed a medium flux/medium resolution instrument to fill a current capability gap in the Western Hemisphere between the high flux wide Q diffraction / total scattering instrument NOMAD and the high-resolution powder diffraction instrument POWGEN. The Powder Diffraction Working Group at the Second Target Station (STS) Workshop held in October 2015 named the instrument concept its top priority for the First Target Station. More recently, the inaugural Powder Diffraction Suite Review Committee, meeting in the summer of 2016 to review ORNL's Powder Diffraction programs, concluded as a leading statement in their executive summary, ***"Our strong recommendation is to construct a rapid acquisition but medium-resolution quiet and stable diffractometer at BL-8 on the FTS as quickly as possible… Such an instrument will restore the US lead in PDF studies of nanostructure, while filling an important gap in our capabilities for in-situ/in-operando studies and should be constructed with all haste."*** The DISCOVER Beam Line Workshop, held May 3-4, 2017, and sponsored by ORNL's Neutron Sciences Directorate (NScD), was convened to define the science goals, instrument concept, and design requirements for DISCOVER, to review preliminary engineering and neutronics calculations, and to outline a preliminary beamline development proposal for NScD management. The workshop was attended by an international committee

of physics, chemistry, and materials science experts, as well as key personnel in neutron diffraction and neutron instrumentation.

Technical Description

The science case for DISCOVER requires the high wavelength resolution provided by a shallow-poisoned water moderator for increased neutron flux in combination with a moderate length incident flight path, a straight guide illuminating the sample homogenously, wide-angular detector coverage, and primary/secondary collimation for low and stable background scattering. Key instrument characteristics are provided in Table 1. In fiscal year 2018 the Neutron Scattering Directorate at ORNL performed an initial scoping exercise on the DISCOVER beamline project to aid in community deliberations and advocacy, including an engineering layout for the instrument, neutronics performance evaluation of various design options, a preliminary Work Breakdown Structure (WBS), and a cost estimate. The current concept for the instrument layout is shown in Figure 1.

Table 1. Key parameters of DISCOVER.

Parameter	Description
Moderator	300 K de-coupled H_2O
Sample size	1.0 cm diameter; 1 to 2.5 cm tall (and smaller)
Moderator–sample distance	32 m
Sample–detector distance	1 - 2.5 m
Wavelength range	0.5 Å $\leq \lambda \leq$ 5 Å
Resolution	$\Delta d/d = 0.2\%$
Detectors	0.8 cm diameter ^{3}He linear position-sensitive detector

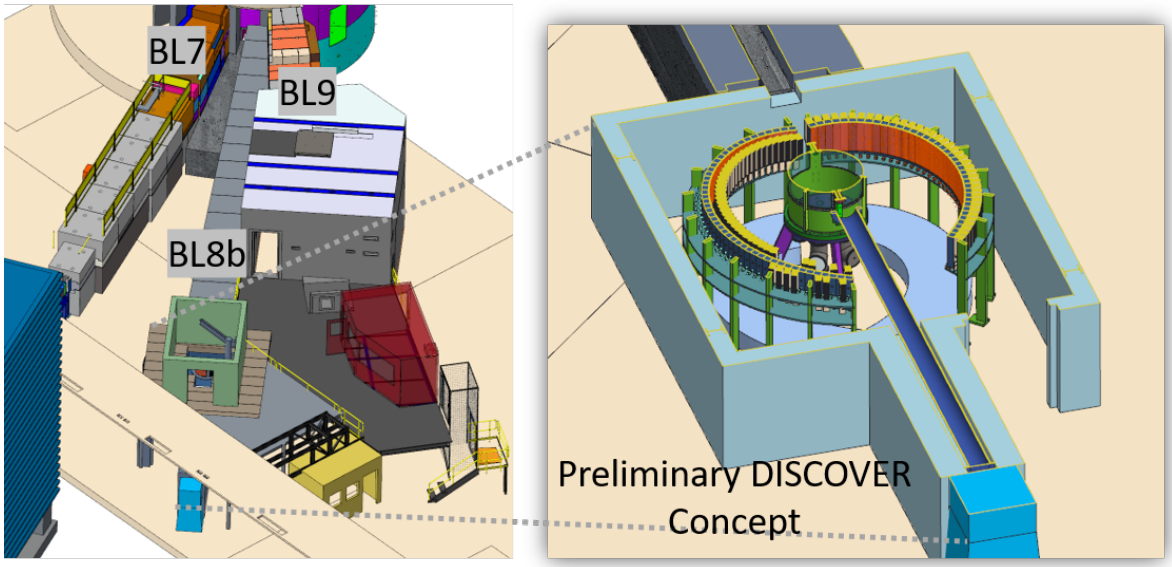

Figure 1. The DISCOVER beamline is currently envisioned to be located on BL8b at the SNS, between Vulcan on BL7 and Corelli on BL9. Preliminary concepts are based on ~32 m primary flightpath, wide angular range and fully collimated detector coverage, and a top-loading sample chamber. The design currently features a full complement of 3He detector tubes located on both sides of the sample chamber in a logarithmic spiral arrangement, with both coarse and fine radial collimation. Access to the sample chamber will be from above, with a top-loading sample well that will accept the current TOF diffraction sample environment suite. Provisions are being incorporated to accommodate an elevating sample platform that will allow access to user-provided sample environments, a feature strongly advocated for by the community at the DISCOVER Beamline Workshop.

Vulcan (SNS FTS beam line 7) has demonstrated the suitability of the shallow poisoned, 300 K water moderator to produce outstanding powder diffraction measurements providing $\Delta d/d = 0.25\%$ in its high resolution (low beam divergence) mode with detectors at 90 deg 2θ. This moderator produces pulses with FWHM of 10.6 μsec at $\lambda = 1$ Å, which should provide better $\Delta d/d$ at higher scattering angles for an instrument with a total flight path of ~32 m. Due to its coupled PDF mission, the instrument must deliver a sufficiently wide wavelength band to cover a broad range of Q-space in a single instrument setting. It is also desired that the instrument resolution function maintain a Q-dependence that is tractable for high real space range modeling. The current concept assumes a full complement of ^{3}He detector tubes located on both sides of the sample chamber in a logarithmic spiral arrangement, with both coarse and fine radial collimation. Performance estimates are being evaluated with the neutron ray-trace simulation package McSTAS to evaluate chopper, guide, and detector layouts, and benchmark these within the performance metrics of the NOMAD and POWGEN beamlines. Several MCSTAS comparisons are shown in Figure 2. Current performance estimates are up to 30 times higher count rates compared to POWGEN, with double the resolution of NOMAD over a large portion of the angular range. With these characteristics, data sets for Rietveld and PDF analysis will be collected for ~1 gram samples in minutes to an hour, depending on scattering strength. Options for detector arrangements, guide characteristics, and chopper arrangements are in progress, and will be determined during a detailed design stage. The current design assumes detectors will operate in an air or Ar-filled environment within the shielding cave; however, a lower background option which locates the sample and detectors within a single, large vacuum vessel is still being considered. Efforts are currently underway to evaluate the feasibility for initial designs or upgrade paths that would allow optional correlation chopper use for removal of inelastic scattering signal and optional polarization capabilities for magnetic diffraction/PDF studies.

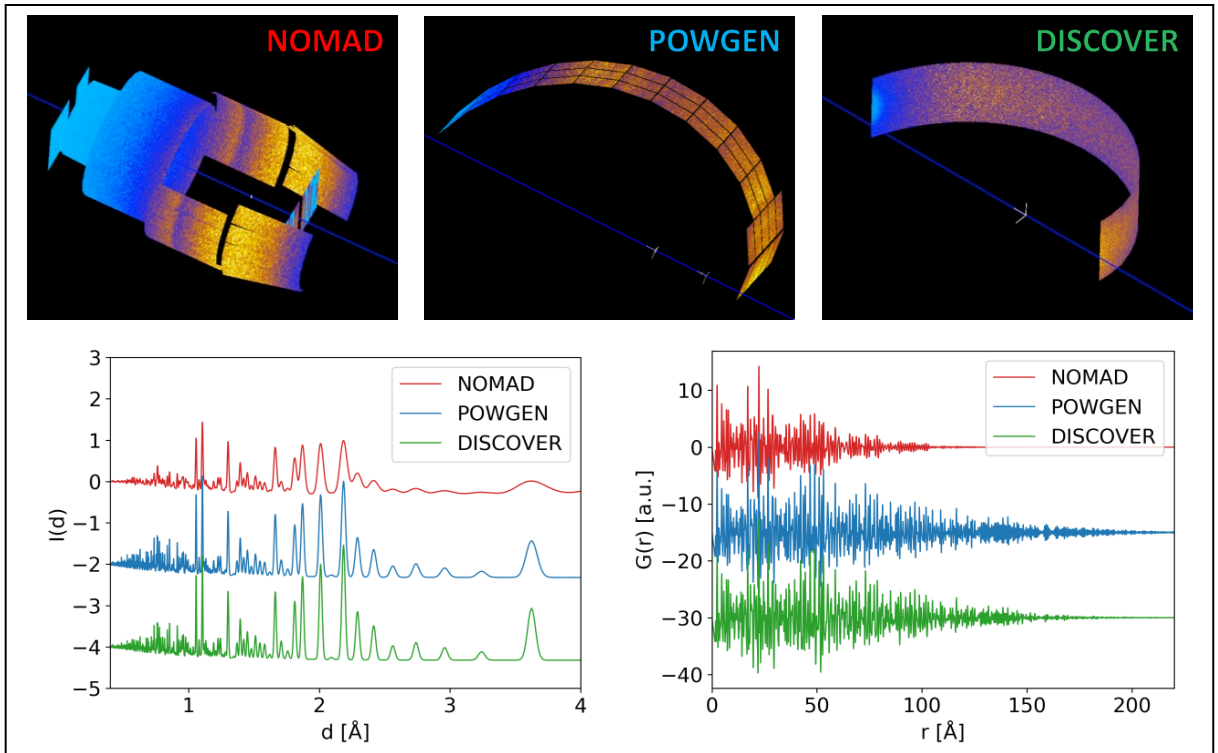

Figure 2. Simulated diffraction intensities and PDFs generated from results of McSTAS simulations within the SNS Powder Diffraction Suite. Simulations are being benchmarked with measurements in the current suite as part of a full design effort.

Summary

We have identified a need and proposed an initial concept for the instrument DISCOVER, ideally placed at beamline 8B at the Spallation Neutron Source, ORNL. The instrument will provide a front-line capability addressing the **Grand Challenge** of "*How do we design and perfect atom- and energy-efficient synthesis of revolutionary new forms of matter with tailored properties*?" put forward in the *Directing Matter and Energy* 2007 report and echoed in a multitude of *Basic Research Needs Reports and Brochures* since. DISCOVER will deliver a medium resolution / fast diffraction capability for kinetic studies of crystalline solids, and it will be the world's highest resolution dedicated *total* scattering instrument; the *total* scattering holds the key to simultaneously determine the crystallographic average structure as well as the local and intermediate (~15 nm) structure often driving chemical and physical behaviors of materials. The instrument will allow the scientific community to advance the state of knowledge of reaction pathways and mechanisms for new material designs, develop new and more effective sorbents and catalysts for the biofuel and other chemical processing industries, identify new paradigms for controlling emergent states of matter in quantum and other functional materials areas, and much more.

2.3 SNS BL-10 – VENUS – a time-of-flight neutron imaging station

Abstract

VENUS will be a world-class neutron-imaging instrument that will utilize the wavelength discrimination provided at the pulsed SNS in novel ways to measure and characterize large-scale and complex systems. VENUS will be an instrument optimized for the measurement of microscale structures utilizing both radiography (i.e., 2D) and computed tomography (i.e., 3D). This novel (to SNS) capability bridges multiple length and time scales to understand, predict and control properties of novel functional materials.

Science Case

VENUS will provide academia, industry, and government laboratories with the opportunity to advance scientific research in advanced manufacturing methods such as advanced nuclear energy systems, additive manufacturing, energy (i.e. electrical energy storage), materials, transportation, engineering, industrial technologies, geosciences, plant physiology, and biology.

Numerous academic and industry research projects have benefited from the existing CG-1D imaging beam line at ORNL's HFIR cold guide hall. Utilizing the capability are major universities, such as Princeton University, University of California-Berkeley, Georgia Institute of Technology, and Brown University, and manufacturers and industry leaders, including Ford, GM, Chrysler, Toyota, United Technologies Research Center, Honeywell, Cummins Engines, Detroit Diesel, Mack, Delphi, Navistar, PACCAR, John Deere, Caterpillar, Volvo, GE, Whirlpool, DuPont, Thermacore, and Bush. These projects have shown the importance and potential impact of world-class neutron-imaging capabilities.

VENUS will be capable of investigating the microstructure of advanced materials including crystalline plane orientation, grain orientation, strain, and in situ mechanical and physical behavior in samples under loads across large regions of interest (field of view of ~20 cm × 20 cm). The beamline will also enable 3D mapping of chemical composition in materials (e.g., nuclear fuels) containing elements that exhibit resonances at short neutron wavelengths (i.e., a few mÅ) and high spatially resolved (~25 μm) neutron radiography over a 2.8 cm × 2.8 cm field of view.

VENUS will be used to evaluate materials at different stages of manufacturing to improve process design and increase efficiency. For example, understanding the composition and microstructure of alloys and the impact of impurities on material properties can be achieved through neutron imaging to determine the spatial distributions of alloying materials; magnetic properties; stress/strain; phases, and the distribution, sizing, and identification of inclusions and impurities. This instrument will particularly excel at measuring interfaces and thin samples. VENUS can also enable the study the behavior of advanced nuclear materials under extreme environments. It may provide insights on how to design and process superior nuclear materials to meet the future energy needs of the United States. VENUS will also contribute in the understanding of properties and processes in complex and heterogeneous subsurface mineral assemblages comprised of porous rock formation, complex fluids that reside within the formation across multiple length and time scales. Advancing the construction of more protective and durable infrastructure, VENUS will enable the study and development of concrete and composite materials with superior mechanical strength. For example, ORNL researchers in collaboration with the Department of Homeland Security recently used neutron computed tomography to quantify the hydrous and anhydrous phases of ultra-high-performance concretes for improved understanding of composite behaviors under normal and extreme environments, such as impacts and fires.

Technical Description

VENUS will be optimized for time-of-flight imaging techniques, such as those available in the general user programs at Japan's J-PARC and the UK's ISIS facilities, but which are currently unavailable in the United States. It will also perform white beam (i.e., continuous source, no neutron wavelength discrimination) attenuation-based measurements when necessary for optimization of TOF measurements. Beam line 10 provides the high neutron wavelength resolution across the cold-to-epithermal spectral range required by VENUS. Figure 1 shows a view of the instrument as installed on this beam line. Table 1 lists in prioritized order the Day 1 technical capabilities provided by VENUS and supported by a suite of integrated data analysis software. Table 2 lists the key parameters of VENUS.

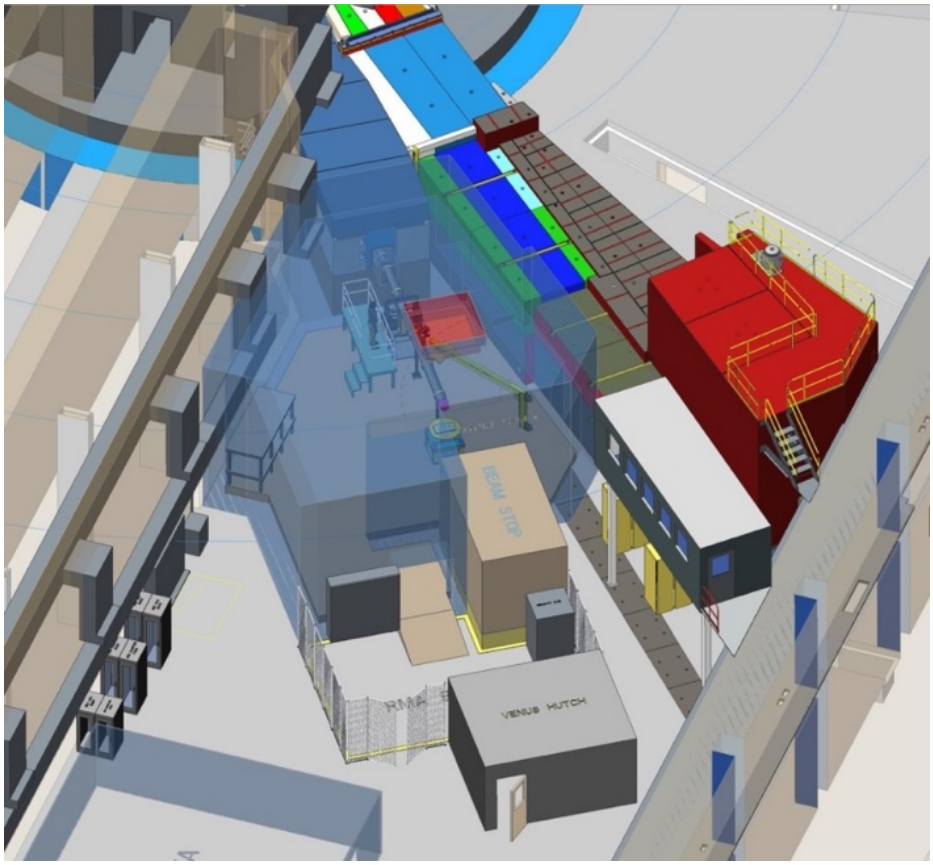

Figure 1. Schematic view of the VENUS imaging instrument concept. The instrument cave, with the ~ 1,000 sq ft floor coverage needed for large samples and sample environments, appears in transparent blue.

Table 1. Day 1 capabilities of VENUS.

Capability	Description
Bragg edge imaging	This technique requires the highest wavelength resolution ($\Delta\lambda/\lambda \sim 0.20$ %) in the thermal and cold neutron range to map Bragg edges in a crystalline structure. The data will assess microstructure properties such as crystalline plane orientation, grain orientation, and/or strain.
Energy resonance imaging	Some elements exhibit isotope-specific resonances at neutron wavelengths of a few mÅ (energies from eV to keV), which can be used to quantify the presence of a particular isotope map in 3D.
Low-resolution energy selective (i.e., time-of-flight) neutron radiography and tomography	For these measurements, a wavelength resolution $\Delta\lambda/\lambda \sim 5$–10% may be sufficient, as the goal is to increase contrast sensitivity.
Epithermal imaging	Epithermal neutrons can be used to provide higher penetration capability in samples that have low transmission in the thermal and cold ranges. This technique trades contrast sensitivity for higher penetration capability.
Stroboscopic imaging (i.e., cyclic motion)	Samples with repetitive motion, which can be tuned to a multiple of the SNS repetition rate, can be imaged using very short time bins (i.e., a few μs) over a total data collection period of several hours.
Conventional attenuation contrast (i.e., white beam) neutron radiography and computed tomography	This is the most common imaging technique and is similar to the normal operating mode of a reactor-based neutron-imaging facility. The contrast is based on the attenuation (i.e., scattering and absorption) of a sample in front of the detector, creating a shadowgraph.

Table 2. Key parameters of VENUS.

Parameter	Description
Moderator	20 K decoupled, poisoned hydrogen
Field-of-view	20 cm × 20 cm (full illumination)
Moderator–sample distance	25 m
Sample–detector distance	A few mm to 10s of cm
Wavelength range	Epithermal to cold
Wavelength Resolution	$\Delta\lambda/\lambda \leq 0.15\%$
Detector	Cameras (CCD and CMOS); Micro-Channel Plate (MCP)
Spatial resolution	50 μm or better with CCD/sCMOS, ~ 25 μm with MCP

2.4 SNS BL-16A – BeFAST, Beryllium Filter Analyzer SpecTrometer

Abstract

BeFAST, a filter spectrometer on BL16A, will complement the dynamic range of energy transfers available at the exisiting VISION (BL16B) instrument. A filter spectrometer uses the transmission of Be or BeO to define a rather broad final energy acceptance (up to 5 meV). The compact nature of the spectrometer results in large solid-angle coverage overcoming the limitations that crystal-analyzer spectrometers like VISION experience in the higher energy transfer region. Although VISION collects data from 0 to 8,000 cm^{-1}, little to no intensity is available above 3,000 cm^{-1}, and extremely long counting times are required to collect useful data in this range of energy transfers. This region of the vibrational spectrum contains chemical bond stretches, which are important to the identification of functional groups and their chemical transformation in chemical reactions. For example, this energy range is important in catalysis in the identification of C-H bonds. BeFAST will be built at the FTS, next to the VISION spectrometer. BeFAST is anticipated to collect data ~5,000x faster than VISION in the region of the spectrum above 2,000 cm^{-1}. Figure 1 illustrates the complementarity between VISION and BeFAST.

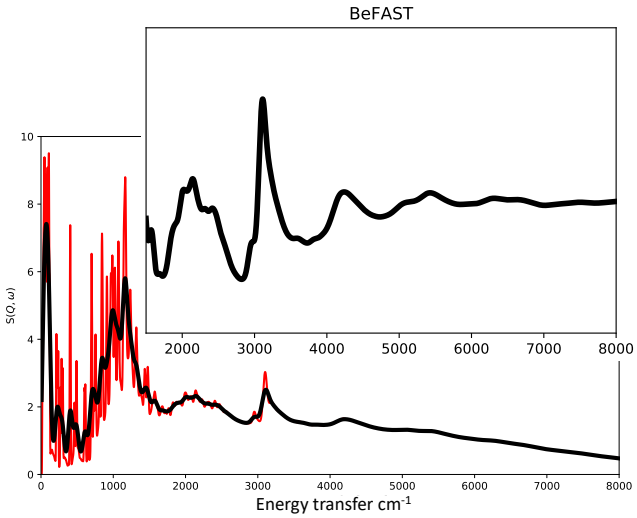

Figure 1. The INS spectra for triphenylmethane calculated for VISION (red) and BeFAST (black), modeled with ICEMAN. Insert, the spectra from 1800 cm^{-1} as calculated for BeFAST.

Science Case

Besides complementing VISION, BeFAST will also allow for new avenues of scientific research at SNS by enabling neutron near-infrared (NIR) spectroscopy. The frequency range above 4,000 cm^{-1} (NIR) is particularly rich in overtones and combination bands. These transitions occur in large part because of bond anharmonicity. Bonds involving hydrogen and some other heavier element such as oxygen, carbon, nitrogen, or sulfur (i.e., O-H, C-H, N-H, and S-H bonds) tend to present high anharmonicity and high bond energy with fundamental vibrational transitions in the 3,000–4,000 cm^{-1} range. It follows that overtones and combinations of the fundamental vibrations of such bonds occur in the spectral range associated with NIR. This energy range is of interest to members of the catalysis community, since many catalytic reactions involve making and breaking C-H bonds, which have stretching frequencies in the 2,800–3,300 cm^{-1}, and many oxide surfaces (and alcohols) have -O–H stretches in the 3800–3500 cm^{-1} region. As the science case for BeFAST is developed, it will be important to engage the catalysis community to ensure this instrument addresses this critical science theme.

The extraction of reliable anharmonic parameters is important for *computational chemistry*, for example in the development of force fields for molecular mechanics or to refine approaches to the reliable computation of vibrational spectra and properties depending on the vibrational density of states. Currently, insufficient experimental data are available, and optical selection rules limit the usefulness of Raman or Fourier transform infrared spectroscopy, particularly with small, highly symmetric molecules. Neutron NIR spectroscopy is not subject to this constraint. Accurate anharmonicity information will also

allow researchers to calculate accurate potential energy surfaces, a conceptual tool used in the analysis of reaction dynamics. Such calculations for realistic reactions and models is now within the reach of supercomputers, and experimental NIR neutron vibrational data will be needed to develop this important field of reaction dynamics. Co-located optical spectroscopy and theory/modeling capabilities at CNMS will add additional value to the instrument's user community.

An important scientific area that would benefit greatly from the availability of neutron NIR vibrational data is *water and other hydrogen-bonded systems*. Water is present in materials in many forms. Its structure and dynamics, whether in the pure state or in various other forms, continue to be the object of numerous studies. Because of strong hydrogen bonding, water is strongly anharmonic. Access to a filter spectrometer with usable intensity in the NIR will provide information on water anharmonicity to researchers in the fields of biology, chemistry, geology, environmental science, and materials science. More generally, anharmonic, hydrogen-bonded molecular entities are associated with important physical behaviors such as glass formation or energy transfer and localization in proteins.

Technical Description

BeFAST is a compact filter spectrometer that can be located in the confined space at the SNS beam line 16A, neighboring the VISION spectrometer. Optimized for higher energy transfers than VISION, BeFAST is anticipated to out perform VISION by ~5,000 for energy transfers > 2000 cm^{-1}. Using this scaling, BeFAST will collect data as fast as 10 minutes from 500 mg of hydrogeneous sample. Table 1 lists the key parameters of BeFAST.

Table 1. Key parameters of BeFAST.

Parameter	Description
Moderator or Beam Line	Water, SNS BL16A
Sample Size	5 cm (V); 3 cm (H)
Moderator-sample distance	~30 m
Sample-detector distance	~0.7 m
Wavelength or Energy Range	10-1,000 meV
Resolution	$\Delta\omega/\omega \sim 2\%$
Detector	^{3}He linear position sensitive, 8 mm diameter

2.5 SNS BL-TBD – HiResPD – high-resolution powder diffractometer

Abstract

The detail that can be learned from crystallographic studies of materials with complex structures is often limited by the resolution of the data. Currently, the highest resolution neutron powder diffractometers in the world are HRPD at ISIS ($\Delta d/d$=0.04%) and SuperHRPD at JPARC ($\Delta d/d$=0.035%). The history of high scientific productivity at HRPD and current synchrotron instruments where this resolution has become standard makes a strong case for having an instrument of comparable neutron performance in North America.

Science Case

Neutron diffraction has greatly enhanced our knowledge of strongly correlated materials and remains one of the principal tools for the determination of magnetic structures. The following two examples highlight the need for higher resolution as the research drive is toward increasingly complex systems.

Example 1: Domain formation has a long and rich history in magnetism and is often critical to the properties of magnetic materials. Recently, magnetic domains with topological properties (e.g., Skyrmions) have risen to the forefront of research of magnetics/spintronics and topological phases of matter [1,2]. While small ferromagnetic domains can be detected and studied using real-space techniques such as Lorentz transmission electron microscopy, the nature of antiferromagnetic domains remains less well understood. A neutron powder diffractometer with exceptionally high resolution at low Q / large d spacing, would lend itself to the study of antiferromagnetic domain behavior.

In a recent series of experiments on the non-centrosymmetric ceramic, $Fe_3PO_4O_3$ (space group $R3m$), it was shown that the material hosts an unusual helical (or conical) antiferromagnetic structure that organizes into small, needle-like domains (~7 nm in hexagonal *ab* plane; resolution limited out of plane; [3]). In this particular case, POWGEN at the SNS could detect finite size broadening of the AFM domains, but only because of the unique materials properties. In general, details of AFM domains (such as their average size, growth characteristics) have been reported in very few materials, owing to the challenge of their measurement. The primary methods used for their characterization include polarized neutron tomography [4], optical second harmonic generation [5], and photocorrelation spectroscopy [6,7]. The microscopic origin of antiferromagnetic domain formation is poorly understood, as there is no demagnetization energy cost; instead, magnetostriction has been implicated in its origin [8,9]. Given a neutron powder diffractometer with exquisite resolution, AFM domains may be detected and studied in other complex magnetic materials in order to be exploited in future technologies. For example, the anisotropic magnetoresistance of antiferromagnetic FeRh has been utilized for a new spintronic device concept [10].

Example 2: Due to their structure and electronic properties, transition metal oxide Ruddlesden-Popper (R-P) phases, and in particular nickel-based R-P phases, provide model systems for high temperature cuprate superconducting compounds, and indeed have been predicted to be potential hosts for superconductivity. Although not superconducting, $La_4Ni_3O_{10}$ (LNO), the n=3 member of the R-P series $La_{n+1}Ni_nO_{3n+1}$, exhibits a weak feature in its electrical resistivity, assigned to a metal-to-metal transition at ~140 K, accompanied by a clear heat capacity anomaly. Theoretical considerations have attributed it to a fermi surface driven charge-density wave; however, the origin of this phase transition remains an open

question. The potential for CDW, stripes, etc. as 'intertwining' orders with superconductivity motivates this work.

Understanding the relationship between the structure of LNO above and below the transition is an essential step toward a comprehensive picture of its physics. Remarkably, even the room-temperature structure of LNO is not without controversy, with reports of orthorhombic *Fmmm* or *Cmca*, or monoclinic $P2_1/a$, or even lower symmetry [11-13]. The differences among these proposed structures are subtle, involving rigid rotations of Ni-O octahedra. The sensitivity of neutrons to oxygen atoms as well as the high resolution provided by a HiResPD instrument will play crucial roles in definitively establishing the correct structure of this nickelate through its metal-to-metal transition.

Complex Chemical Systems:

Functional materials of scientific and technological interest, such as zeolitic solids, piezoelectrics, controlled thermal expansion materials, ionic conductors, etc., commonly display a high level of crystallographic complexity (very large unit cell volumes) and/or subtle structural distortions. In many cases, this structural complexity is integral to the useful physical properties of the materials. To properly address such problems using powder diffraction, high resolution data is needed both to resolve subtle splitting in peaks and/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.

Neutrons due to their sensitivity to light (low-Z) elements have been a tool of choice for the characterization of Li-ion battery materials. Despite their great advantage, safety has always been a major concern for lithium-ion systems [14] due mainly to the high operating voltage (> 3V) and utilization of ignitable liquid or polymer-based organic electrolytes. The failures of Li-ion batteries are often found to occur during the charging process, when the transition metal ions enter higher oxidation states while Li^+ is extracted from the structure. The delithiated oxide cathode, with large amounts of high-valence transition metal ions such as Co^{3+} or Ni^{4+}, [15] becomes highly activated, such that it may readily be reduced via the release of structural oxygen [16]. This process can result in the oxidation of organic electrolyte, leading to the failure or even explosion of the battery.

One possible mechanism to combat the safety issue in Li-ion batteries is to operate an all solid-state battery, which has a non-flammable solid electrolyte such as $Li_7La_3Zr_2O_{12}$ (LLZO) garnet. LLZO is a fast ion conductor and is chemically and electrochemically stable against metallic Li. Having demonstrated its viability in solid-state batteries, efforts are currently focused on manufacturing and scaling-up synthesis. However, current neutron diffraction analyses carried out at POWGEN [17,18] indicated anomalous crystal lattice effects pointing to inhomogeneous Li and dopant distribution. It is believed that the synthesis conditions, e.g. time, temperature, and atmosphere, affect phase purity, thus resulting in inconsistent conductivity, stability, and mechanical properties. Detection of the subtle changes in the crystal structure and stoichiometry can only be determined with high-resolution neutron diffraction analysis, which is currently absent in the US neutron sources. These types of experiment can be accomplished by using the proposed HiResPD instrument at the STS and highlighted by data in Figure 1, which were collected on a similar resolution machine at the advanced photon source (APS). However,

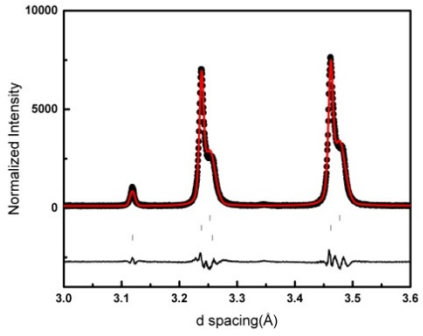

Figure 1. Magnified region of the refinement of synchrotron x-ray diffraction data after convergence for the sample with composition of $Li_{6.5}La_3Zr_{1.5}Ta_{0.5}O_{12}$ highlighting the two cubic phases observed.

even in this latter case, Li distribution in the multiphase sample could not be determined from these high-resolution X-ray data due to the insensitivity to Li and O in the presence of much heavier La and Zr. The ability to measure these subtle effects will bolster efforts to mature LLZO solid electrolyte membrane technology to accelerate the development of higher energy density and safer batteries.

Ab-initio Structure Solution:

The collapse of information from 3D to 1D has always meant that structure solution from powder diffraction data (SDPD) is significantly harder as compared to single crystal diffraction. Nevertheless, with improvements in instrumentation, algorithm development and enhanced computing power, great strides have been made in ab-initio structure solution from powder diffraction. While the contrast afforded by difference is Z often makes X-ray diffraction the method of choice for structure solution, there remain some cases where neutron diffraction is preferred. Indexing and determination of space group is the first step in SDPD and high-resolution data, which provides more precise d-spacing information, is extremely important.

The sensitivity of neutrons to light elements can play a crucial role in the determination of the correct space group. For example, the tilting of TiO_6 octahedra in perovskites or methyl group orientation in small molecules can subtly affect the space group in a manner that is difficult to determine from X-ray data. Neutron data is highly effective when used on framework structures to find the light atoms such as hydrogen, CH_4 or CO_2 inside clathrate, MOF, or zeolite structures using Fourier cycling. Neutron diffraction data can play a critical role in the structure solution of small molecule and organic inorganic hybrids, heavy metal oxides and other more complex compounds. As the demand for complex structure solution from powder diffraction data grows, the need to combine X-ray and neutron powder diffraction will also increase. Ideally that need can be met by having access to a neutron powder instrument which has the same resolution afforded by synchrotron powder beam lines.

Technical Description

HiResPD 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 and physics mission of in situ/in operando measurements across a wide range of temperature and pressure, magnetic field, electrochemical cells, and gas handling systems.

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

Initial concept development for this instrument assumed that it would be illuminated by a decoupled, poisoned moderator STS. Subsequent considerations place these high-resolution moderators on FTS (see Section 1.1). Even without re-optimization of the neutron optics concept, the instrument will have ≈50% the performance it would have had if located at STS (the STS moderator was optimized to produce higher peak brightness and was smaller than the eqivalent FTS moderator). It is expected that the larger FTS moderator will improve the performance above this value, especially for the shorter neutron wavelengths the instrument will use. The neutron guide will start approximately 20 m from the moderator and extend to 7.5 m upstream of the sample position and provide the capability to adjust the beam divergence at the sample from a high flux mode (10 mrad) to a high-resolution mode (1.2 mrad) illuminating approximately 7 x 9 mm^2 sample area. Scaling performance from the original STS concept, HiResPD at FTS in high flux

mode is expected to have a ≈4.5x gain for first frame operation (0.5 Å ≤ λ ≤ 8 Å at 5 Hz; 0.5 Å ≤ λ ≤ 3 Å at 15 Hz) relative to POWGEN. Even in high flux mode, HiResPD will provide better resolution than POWGEN. Instrument resolution is illustrated in Figure 2. The instrument will need multiple bandwidth neutron choppers to enable frame suppression and a 5 Hz mode of operation. A T0 chopper is required to remove high energy neutrons and gammas produced when the proton pulse strikes the mercury target. Figure 3 shows an engineering concept of the instrument end station illustrating the detector layout which follows the same equiangular spiral as used in POWGEN. Table 1 lists the key parameters of HiResPD.

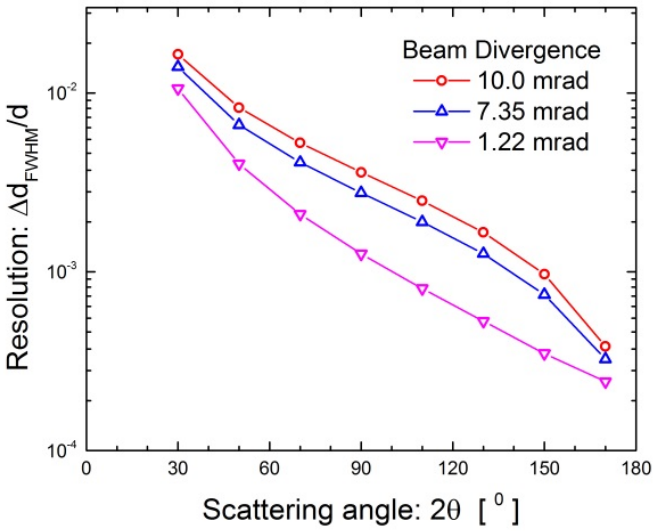

Figure 2. Resolution on HiResPD as a function of scattering angle. As the dependence on wavelength is weak, the data are average values for fixed scattering angles.

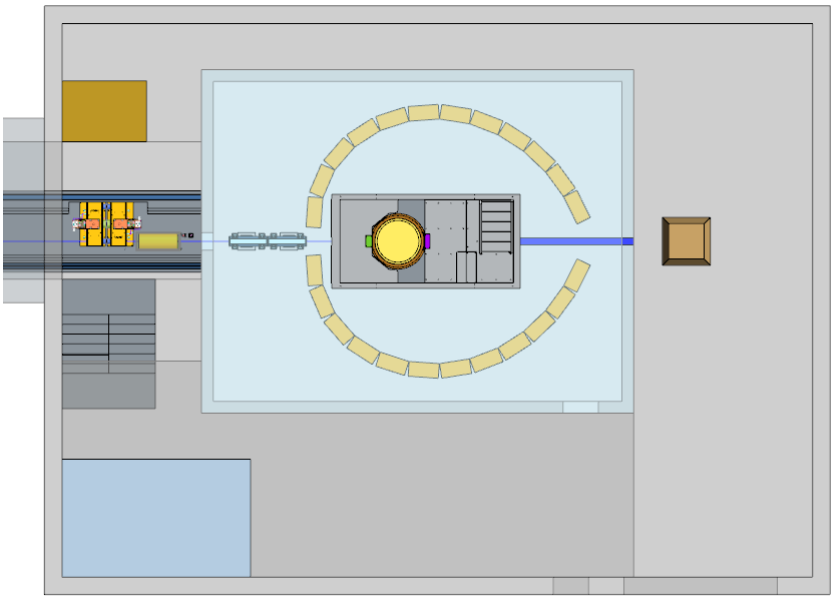

Table 1. Key parameters of HiResPD.

Parameter	Description
Moderator	20 K decoupled, poisoned hydrogen
Moderator–sample distance	100 m
Sample–detector distance	4.75 m (at 10 deg); 2 m (at 170 deg)
Wavelength range	Epithermal to cold
Wavelength Resolution	$\Delta\lambda/\lambda \leq 0.03\%$ (at 1 Å)
Detector	Wave Length Shifting Fiber or ^{3}He

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2.6 HFIR Cold Guide Hall, CG-1 – MANTA, Multiple Analyzer Triple-Axis for HFIR

Abstract

Recent experience has shown the combined strengths of time-of-flight and triple-axis spectroscopy can yield tremendous insight into a diverse set of problems in materials research associated with magnetism, superconductivity, and ferroelectricity. The MANTA instrument will expand this powerful combination into the essential sub-thermal energy regime while increasing overall counting efficiency by two orders of magnitude relative to traditional cold TAS instrumentation.

Combined with the high incident neutron flux, an innovative wide-angle energy-dispersing detection system on MANTA will allow high efficiency measurements with a "footprint" in Q-E space that is complementary to SNS-based time-of-flight spectrometers. MANTA will exploit and extend the most recent advances in focusing optics, multiplexing crystal spectrometers, and neutron polarization methods for a unique new capability to map excitations within a scattering plane over a selectable range of energy transfers. The planar nature of its detector systems will also ensure that MANTA is an ideal instrument for parametric studies with a range of complex sample environments.

Science Case

Inelastic neutron scattering of cold neutrons is uniquely adapted to the discovery and unambiguous understanding of emergent quantum states, ranging from spin-liquids and topological materials to functional heterostructures and mesoscale-ordered materials. Modern time-of-flight spectrometers can produce comprehensive maps of momenta-energy space but require large single-crystals for high signal-to-noise and present challenges with complex sample environments. We propose to combine the high time-averaged flux at HFIR (which is HFIR's niche in the 3-source strategy) with latest advances in neutron optics and polarization methods and a massively-multiplexed detector system for a unique new capability: mapping of the energy-dependence of excitations within a scattering plane in small "as-discovered" crystals of forefront materials. With MANTA's flexibility, giant leap in efficiency, native polarization analysis, and ability to accommodate extreme sample environments, our concept dramatically broadens the range of quantum materials amenable to neutron spectroscopy.

The MANTA cold neutron spectrometer at HFIR will use the latest advances in neutron optics and multi-analyzer configurations for high efficiency measurements over a distinct volume of Q-E space that provides an important complement to SNS instrumentation. Specifically, MANTA will enable:

1. Very high efficiency mapping of Q-dependent scattering within a plane for a select range of energy transfer from 0.2 meV to 15 meV. When the energy range of interest matches the spectral range of the energy dispersive detector, MANTA may provide the highest efficiency of any ORNL instrument.

2. Fully polarized beam capability to separate magnetic and nuclear scattering and detect specific spin components of the magnetic scattering.

3. Through variable Bragg- and guide-based focusing, the instrument can accommodate either a small sample size with relaxed Q-resolution for the multiplexed analyzer configuration, or moderate sample sizes with high Q-resolution employing a more conventional single-scattered path analyzer / detector. Initial operation of MANTA will employ this single analyzer approach.

4. The wide-horizontal angle scattering geometry enables high intensity parametric studies and matches the solid angle available for state-of-the-art pressure cells and high-field magnets.

5. A non-multiplexed spectrometer configuration is well matched to ultra-high-resolution optics employing Wollaston prisms that have already been demonstrated to enhance Q resolution with reasonable count rates; this setup has the potential to measure lifetimes of magnetic and lattice excitations with μeV resolution.

The colocation of SNS and HFIR at ORNL has proven to be powerful scientifically and, for the case of thermal neutrons, there are multiple examples where research groups have combined data from the two sources to enable high profile science. In general, the broad mapping capabilities of SNS instruments, such as ARCS and SEQUOIA, provide an overview of the scattering from a specific material that identifies features of interest, while the high monochromatic flux of thermal triple-axis instruments allows for parametric studies of these features. The combination of the proposed new STS direct geometry instruments and MANTA will expand such complementarity to the cold neutron regime.

Just as new instrumentation concepts are allowing orders of magnitude gains for pulsed source instrumentation, this is also the case for reactor-based instrumentation. The combination of Bragg- and guide-based focusing methods and the multi-analyzer configuration described below allows ultra-high efficiency mapping of inelastic scattering over a range of scattering angles and energy transfers based on the high time average cold neutron flux at HFIR.

One area where MANTA would have transformative impact is in the study of quantum spin liquids. Spawned in the quest to understand superconductivity in transition metal oxides, this area has turned out to be extraordinarily rich and holds promise for applications in quantum computing. Theoretical progress and progress in new materials synthesis indicate the time is ripe for a breakthrough in this area and inelastic neutron scattering will surely play a critical role. However, the bulk scattering cross section can be difficult to interpret because neutrons typically cannot create or annihilate the underlying quasi-particles individually. Theoretical work shows that studying the configuration of spin singlets that form in the vicinity of defects or at the edges of quantum spin liquids can help to determine the nature of the bulk spin liquid state [1]. Neutron scattering can access this pattern by mapping the Q dependence of the inelastic scattering associated with defects in the spin liquid. For localized excitations associated with defects, the influence on scattering exists over a restricted range of energy transfers. The angular coverage of MANTA combined with simultaneous mapping of a range of final energies makes this an ideal instrument to probe the momentum space wave function of bound states in quantum spin liquids.

Many scientific problems can benefit from high efficiency measurements over a restricted range of Q-E space. One problem of current scientific interest is the study of topological states in quantum spin ice. This type of materials is predicted to exhibit power-law “dipolar” correlations that are anisotropic in spin space and decay as r^{-3} in real space [2]. Power-law correlations without a broken symmetry and away from a critical point are remarkable signals of underlying gauge symmetry. After Fourier transformation of these correlations on the lattice, a static spin structure factor with “pinch points” at reciprocal lattice vectors in momentum space is obtained. These “pinch points” in spin ice materials are localized at specific regions of Q space where their signature in neutron scattering is that S(Q) is singular in one direction and diffuse in all others. Extended in momentum space, yet with important sharp features, the elucidation of such scattering requires broad high-resolution coverage of momentum space. Measurements were carried out with a wide-angle thermal spectrometer at Helmholtz-Zentrum Berlin [3] demonstrated the need for these capabilities for a classical spin ice material. The focus is now shifting towards quantum spin ice materials where energy resolution is also required [4]. MANTA could lead the way in this active field of research to probe quantum spin ice and other quantum spin liquids with emergent fractionalized quasi-particles under extreme conditions.

Understanding the role of itineracy in heavy fermion materials is another area where the MANTA spectrometer would have strong impact. Heavy fermion compounds are strongly-correlated materials where interactions between f-electrons and itinerant electrons lead to a Fermi liquid-like state with effective electron masses that are two to three orders of magnitude larger than the bare electron mass [5]. Heavy fermion systems are naturally described in terms of a renormalized band structure with intricate features within meV of the Fermi level [6,7]. Cold neutron inelastic scattering is a critical tool to elucidate such band structure and the associated spin correlations. The relevant energy range is <10 meV, and wide-angle coverage is essential to be able to reconstruct the underlying band structure as demonstrated on SEQUOIA for the topological Kondo insulator SmB_6[8]. Particularly in the fully polarized mode where broad magnetic scattering can be unambiguously separated from nuclear backgrounds, MANTA will open a new window on this fundamentally important class of materials that represent the vanguard in our understanding of strongly correlated electrons.

Another area where wide-angle fully polarized capabilities will be essential is in the study of multiferroics. MANTA will be the optimal instrument for experiments where there is a need to explore specific modes or branches that occupy a limited range of energy transfer as a function of external parameters such as electric or magnetic fields. As competition and interactions between multiple degrees of freedom are of growing importance at the forefront of quantum materials research, expansion of polarization analysis will be essential to separate the distinct components of composite quasi-particles and provide a stronger link to theory.

Finally, MANTA will preserve the flexibility of triple-axis instruments and will include a single analyzer-detector option to allow for ultra-high-resolution measurements. Enabling these ultra-high-resolution measurements with both thermal and cold neutrons will broaden the scientific impact of this technique and allow for studies on a broader range of materials.

Technical Description

By employing a multiplexed approach in both energy and scattering angle, MANTA will emulate both direct and indirect geometry spectrometers as illustrated in Figure 1. By preserving the shielding and collimation of the scattered and analyzed beam for background suppression, MANTA will preserve the best features of triple axis spectrometers. By coupling the high time-averaged cold-neutron brightness at HFIR with high reflectivity ballistic-like guide systems, we can maximize intensity in a small sample volume, both enhancing signal and suppressing background. This combination will enhance the complementarity between the spectrometers at HFIR, the first target station at the SNS, and eventually the second target station.

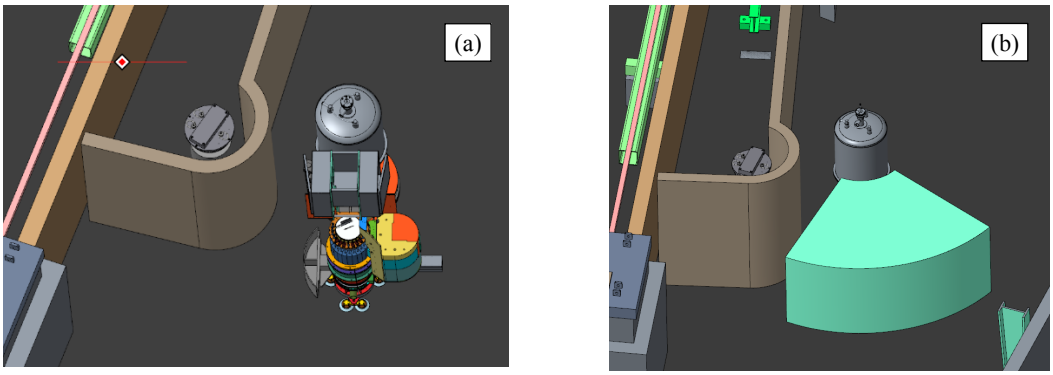

Figure 1. Schematic views of MANTA including (a) the single analyzer-detector option, (b) the multiplexed analyzer-detector option.

The incident beam optics of CG-1 were designed a number of years ago to allow for a vertically-focused beam on a triple-axis instrument with minimal horizontal beam divergence, enabling measurements with high Q resolution. The calculated peak flux on sample for the existing optics configuration was 1.9×10^8 n/cm^2/s (for $E_i = 9$ meV) [9]. The community's need to enable inelastic neutron scattering on smaller samples necessitates a redesign of these optics to provide the highest possible flux on the sample. Fortunately, developments in neutron guides now allow for higher *m* coatings and elliptically focused optics, which can greatly increase flux on the sample while simultaneously suppressing neutron flux near the sample for lower signal and enhanced dynamic range. This requires modification of the near source beam extraction to provide higher beam divergence to the downstream optics, together with an optimized guide design to properly transmit this divergence to the monochromator. As with many modern cold triple-axis instruments, the optics design will include a virtual source upstream of the monochromator and a double focusing PG 002 monochromator. In addition, a velocity selector will be included in the incident beam to eliminate higher order contamination and, thus, reduce background. Comparisons to other instrument upgrade projects internationally [10] indicate that gain factors of five to 10 are possible with such an upgrade and should result in a peak flux in excess of 1×10^9 n/cm^2/s, making the CG-1 inelastic instrument the most intense monochromatic beam of cold neutrons in the world. This should allow for inelastic measurements on milligram samples, making it the ideal complement to the CHESS instrument proposed for STS with the flexibility to also use larger samples when available.

In recent years, significant progress has been made in multiplexing continuous source spectrometers to allow more efficient mapping of Q-E space. At ORNL, it is important to take into consideration complementarity of such an instrument with SNS instruments now and in the future. As such, parametric measurements over a restricted range of Q-E space is a critical strength of inelastic instruments at HFIR that must be preserved. Fortunately, a recent multiplexed design allows for high efficiency mapping while maintaining the ability to measure with high time-integrated flux over a range of Q-E space. This involves using analyzer crystals that scatter vertically, allowing for a nearly continuous coverage of scattering angles (the anticipated range of 2θ coverage would be greater than 160 degrees). The vertical scattering geometry allows multiple final energies to be measured simultaneously by stacking subsequent analyzers behind one another. It is anticipated that at least 10 final energies could be measured simultaneously over this full 2θ range for quasi-continuous angular and energy coverage. The fixed analyzer positions of such a spectrometer simplify motion control so that only the sample and the post sample spectrometer move during measurements. The nearly continuous angular and multiple final energy coverage vastly expands the number of simultaneous Q-E points that can contribute to a parametric study, is perfectly matched with the planar access of extreme sample environments and makes this instrument extremely efficient for mapping planes of inelastic scattering.

The above configuration also will allow for polarized neutron inelastic measurements with sample guide fields along any chosen direction. The incident beam polarization would be accomplished with either a supermirror polarizer or a ^{3}He cell. Post sample polarization analysis could be accomplished with a ^{3}He cell in a PASTIS-type configuration or possibly with a broad supermirror analyzer like the one fabricated for use on HYSPEC. With three orders of magnitude gain in overall counting efficiency, the polarized neutron scattering technique introduced by Moon et al. almost half a century ago [11] would come to full fruition and eliminate the need for the ambiguous methods now used to separate nuclear and magnetic scattering.

Table 1. Key instrument parameters for MANTA.

Parameter	Description
Source/beam line	HFIR Cold Source, CG-1
Energy range	E_i from 2.5 to 25 meV
Energy transfer resolution	0.07–1 meV at $\Delta E = 0$
Sample size range (beam size)	Variable. Samples as small as 10 mg possible
2θ range	>160 degrees
Number of final energies	>10
Detector type (number)	^{3}He single tube (~1,000)—option of PSDs will be considered in instrument optimization

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2.7 HFIR Cold Guide Hall – kSANS, kinetic SANS

Abstract

kSANS is a concept for a high flux, dynamic range SANS instrument optimized for kinetic studies. With plans to operate from the continuous cold source at HFIR, kSANS will be equipped with a velocity selector and chopper system to allow both monochromatic and ToF modes of operation. The versatility afforded by this scheme for a SANS instrument will open many new scientific opportunities with particular advantages for performing new and challenging kinetic measurements. The vision is that kSANS will enable high-impact experiments, especially in biology and soft matter, where a high neutron flux coupled with enhanced time resolution will be most beneficial. Ultimately, kSANS could be moved to the STS, once built, to attain even greater performance.

Science Case

The kSANS instrument will provide the capabilities necessary to conduct innovative kinetic measurements. Simultaneously, the increased neutron flux enables studies of dilute, low contrast, and weakly scattering materials. These benefits will poise kSANS to make significant contributions in the areas of dynamic biological and polymeric materials that are capable of undergoing rapid structural changes. In particular, intrinsically disordered proteins (IDPs) are highly dynamic and do not by themselves fold into well-defined shapes. However, they are essential for many biological processes and highly prevalent in the human proteome. About 44% of human protein-coding genes contain disordered segments (1). IDPs were identified as one of the key new drivers in biological research at the Biology Grand Challenges Workshop held at the University of California, San Diego in January 2014 (2). Establishing relationships between disorder and function is a major challenge, but it is one where neutrons can make substantial contributions due to their unique ability to probe the heterogeneous conformations of disordered systems in solution. With the enhanced time resolution and extended spatial range and resolution of the proposed kSANS, the structural knowledge gained on IDPs and their complexes will provide a framework for understanding the molecular basis of diseases, while providing insights for innovative therapeutics. Particular example cases are:

- *Cellular signaling events*. Understanding the interaction and regulation of the cell adhesion protein CD44 in signal transduction is critical to both cell migration and cancer metastasis. SANS has revealed important signaling requirements for CD44 to assemble into a specific complex necessary for its various functions (3). kSANS will allow the next steps to determine the time evolution of activation and conformational changes. These experiments will yield unprecedented insights into the structural kinetics of highly dynamic biological systems that regulate cell migration and adhesion.

- *Amyloid formation*. A major challenge in neurodegenerative disorders, like Alzheimer's and Huntington's disease, is to identify and characterize the earliest species formed during amyloid formation. Time-resolved SANS is providing new structural information on the aggregation of mutant huntingtin, the protein responsible for Huntington's disease, (4, 5). kSANS will dramatically improve the time resolution for such studies and, with a broader simultaneous length-scale coverage (Q-range), provide a more detailed picture of the early structural evolution. Such kinetic measurements are likely to be essential toward developing potential therapeutics to combat these disorders.

- *IDP phase separation kinetics*. Networks of IDPs can form distinct fluid phases within the cell, referred to as membrane-less organelles. SANS has proven to be a powerful tool in characterizing nucleolus-like liquid-liquid phase separated systems (6). Similar approaches now can be applied to other membrane-less organelles. In particular, kSANS will allow fast, time-resolved measurements of structural changes that occur during pathological "aging" of

membrane-less organelles as relevant to certain neurodegenerative diseases. This capability would help efforts to develop small molecules that inhibit or even reverse the aging process.

Additional kSANS science areas include steady-state and driven flow, polymer processing, synthesis science, and complex and highly ordered materials. Also, with the flux of kSANS, its throughput will be well-suited to help support a SANS mail-in program.

Technical Description

kSANS will complement the current ORNL SANS suite as a versatile HFIR instrument optimized for kinetic studies (see Figure 1). By leveraging the flux at HFIR, kSANS will have both a velocity selector and chopper system to convert between monochromatic and ToF operation modes. Some advantages of ToF for a reactor SANS have been demonstrated by D33 at the ILL, where the pulsed wavelength band increases the dynamic Q-range and can offer tighter and more flexible wavelength resolution options compared to a velocity selector (7). Also, kSANS satisfies several community recommendations:

- "Develop technologies that allow more rapid data collection for time-resolved studies of kinetic processes." *–Biology Grand Challenges Workshop, San Diego, 2014* (2).

- "The committee urges ORNL to consider building further SANS instrument(s) on the HFIR source" – *Review of the Instrument Suite for SANS/Reflectometry at SNS and HFIR, 2017* (8).

kSANS will have a variable sample-to-detector distance from 1 to 10 m and available wavelength range from 4 to 20 Å to yield an accessible Q-range of about $0.002 \leq Q \leq 1$ Å^{-1}. The wavelength resolution will be variable with minimum $\Delta\lambda/\lambda = 10$ and 2% for the monochromatic and ToF settings, respectively. The ToF mode affords narrow wavelength bands, making kSANS a good platform for GISANS experiments. kSANS also will be compatible to provide other setups, like TISANE and MIEZE. Enhancements over current SANS instruments will include optional Wolter focusing (9) within the variable collimation scheme and a 350 µ resolution (thin) detector. The use of multiple detectors, either like D33 at ILL or CG-3 at HFIR, should be considered. Overall, kSANS could potentially perform 50x faster for "traditional" SANS samples, compared to present SANS. While the dramatic reduction in data collection times translates to higher sample throughput, the greater incident beam flux also can be traded for smaller sample sizes. Samples can be 1 to 16 mm in diameter. This is a useful consideration that is especially important for some difficult-to-obtain biological materials. Sample environments will be designed to specifically optimize time-resolved experiments on kSANS. Stopped-flow and continuous-flow devices would support controlled mixing in-beam. Multi-modal setups and rheo-SANS also will be accommodated. In general, kSANS will have a versatile sample environment area capable of mounting large equipment, like magnets and cryostats. Table 1 lists key parameters of kSANS.

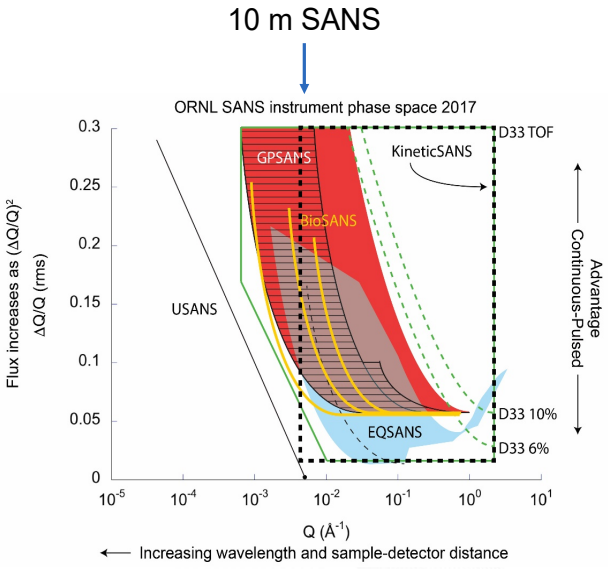

Figure 1. Schematic of the estimated kSANS Q-resolution vs. Q-range compared to the existing ORNL SANS instruments and D33 at ILL. Image courtesy of M. Fitzsimmons (ORNL).

Table 1. Key parameters of kSANS.

Parameter	Description
Moderator	HFIR Cold Source, TBD
Sample size range (beam size)	1 to 16 mm (diameter)
Moderator-sample distance	To be determined
Sample-detector distance	1 to 10 m
Wavelength/Q range	$4\ Å \leq \lambda \leq 20\ Å$ $0.002 \leq Q \leq 1\ Å^{-1}$
Resolution	$\Delta\lambda/\lambda$ = 2 to 10% (variable)
Detector	^{3}He linear position sensitive

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2.8 HFIR Cold Guide Hall –NSE at HFIR, High Resolution Neutron Spin Echo Spectrometer at HFIR

Abstract

This will be a new, IN-15 type, high resolution spin echo spectrometer optimized for long wavelength neutrons, λ~8 Å and greater, to enable the best energy resolution that known technology can achieve. A high-level goal is to reach a correlation time of ~500 ns which will require λ~18 Å wavelength. After the planned upgrades of the cold source and the cold guide systems at the High Flux Isotope Reactor (after ~2024), the new NSE instrument will be placed at a new guide end station. The beam will be designed such that it will be converging on a relatively small cross section at the sample position, ~1-2 cm^2 area, which will enable studies of smaller samples. This will address the needs of the biological and medical communities by allowing the investigation of important biomolecules for drug research and drug delivery, that can be purified and deuterated in small quantities only, as well as to other research area of soft condensed matter like organic photovoltaics, biomimetic materials and polymeric membranes. This design feature will also be beneficial for studying the slow correlations in hard matter and new quantum materials. The advantage of HFIR relative to the planned STS will be that one can deliver a much less monochromatic beam to the sample, δλ/λ~15%, enhancing the useable intensity. The relative merits of an NSE instrument at HFIR with time-of-flight option, and one at STS with reduced δλ/λ will also be studied.

Science Case

In a recent report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science" [1], DOE's Basic Energy Sciences Advisory Committee (BESAC) reviewed recent progress on general topics identified in an earlier report [2], and formulated five "transformative new opportunities" for basic research in energy science. Two of these, "Mastering Hierarchical Architectures and Beyond-Equilibrium Matter", and "Beyond Ideal Materials and Systems: Understanding the Critical Roles of Heterogeneity, Interfaces, and Disorder", can be addressed through the study of slow dynamic correlations, on multiple time scales, with neutron spin echo spectroscopy. A new instrument, designed to conduct such studies in a wide range of new materials and systems, will be proposed for the cold guide hall at HFIR. This instrument will greatly enhance neutron scattering capabilities at ORNL in the area of high-resolution quasi-elastic scattering. Specifically, this will include the following scientific research areas.

- slow dynamics in complex organic molecules relevant for biological function
- surface excitations, dynamics on liquid surfaces or of membranes at low Q
- liquids, polymeric systems, colloids, gels
- diffusion in protonic and ionic conductor materials
- dynamical processes in new quantum materials in a wide range of time scales
- geometrically frustrated magnets, stripe order materials, skyrmion lattices
- materials with complex energy landscape, hierarchical arrest/relaxation

Example 1 – Dynamics of Membranes in Living Cells

Modern spectrometers have sufficient sensitivity to directly probe the mobility of intracellular photosynthetic membranes in living organisms. Biological function of proteins is intimately coupled to conformational changes and internal dynamics. Neutron spin echo has already proved to be a successful method of studying the structure and dynamics of model bilayer lipid membranes and proteins in solution, that is, on model systems under defined experimental conditions. It is now possible to perform such studies with the membranes in their natural, complex environment of a living cell. A recently published

high-resolution inelastic neutron scattering study on the cyanobacterium Synechocystis sp. PCC 6803 assessed the flexibility of cyanobacterial thylakoid membrane sheets and its dependence on illumination conditions [3]. It was observed that thylakoid membranes in the dark are softer and show three- to four-fold excess mobility compared to membranes under high light conditions. The study shed new light onto the potential role of lipid bilayer membrane dynamics in life-sustaining processes such as photosynthesis.

Example 2 – Stripe Order Materials
Spin freezing is one of the most common but least understood regimes of spin ordering in magnetic materials. Unlike conventional ordering, which results in the long-range magnetic structure and appearance of elastic magnetic scattering and Bragg peaks, spin freezing results in a short-range order characteristic of a correlated glass. This order appears static in a conventional neutron scattering experiment, but the ultimate energy resolution offered by spin echo spectroscopy allows one to approach the critical temperature and reveals subtle dynamic features in the glassy phase itself. Recently, correlated glassy states and the corresponding freezing transitions have been studied in the layered transition metal oxides $La_{2-x}Sr_xCoO_4$ at well-defined values of x [4]. These materials show static stripe-like charge order similar to the hole-doped copper oxide superconductors, where it competes with superconductivity. In the Co-based systems, it is found to co-exist with short-range, quasi-one-dimensional, antiferromagnetic order, which may provide a natural explanation for the distinctive hourglass shape of the magnetic spectrum previously observed in $La_{2-x}Sr_xCoO_4$ and many hole-doped copper oxide superconductors. Neutron spin echo offers the resolution necessary to reveal the dynamics of the magnetic correlations in the stripe phase, which may form the basis for a better understanding of these materials.

Technical Description

The highest priority for ORNL is to reach the best possible energy resolution with the available technology. Therefore, the instrument will be of the generic IN11/IN15 type with long solenoidal precession coils. Preliminary design studies will be performed in the near future that address the following three technical question in particular.

1) What should the guide system look like that delivers neutrons to the sample position. The optimization should be for long wavelength neutrons, $\lambda \sim 8$ Å and greater. It is also desirable to focus the beam at the sample position into a relatively small area. Spin echo can tolerate a relatively large beam divergence at the sample position. It will be studied whether a paraboloidal mirror can provide, under these conditions, an intensity gain at the sample over a more conventional guide. The guide exit would be relatively far from the sample position, ~4 meters minimum.

2) To deliver neutrons in a desired wavelength range to the sample, should the instrument use a velocity selector, a chopper system (like D33), or both. A velocity selector is the conventional choice for wavelength selection at a reactor source, because the wavelength distribution $\delta\lambda/\lambda$ can be chosen to be large, ~15%, and independent of wavelength. Time-of-flight would allow one to choose a wider wavelength band $\Delta\lambda$, but at the cost of $\delta\lambda/\lambda$ becoming smaller for longer wavelength, which costs intensity. The design of the D33 (ILL) chopper system was an attempt to overcome this limitation for the specific case of a SANS instrument, which differs from spin echo in that the detector location is variable. The exact implications of a time-of-flight option for a spin echo instrument at HFIR will be studied, which will facilitate a performance comparison with a similar instrument concept at STS.

3) Should the precession coils be superconducting or should they be conventional water-cooled copper coils. The technical development of superconducting coils for use in spin echo

instruments has been pushed by the Jülich group. These coils can be more compact, and the accuracy of the windings can be better than with normal conducting copper wire. These are desirable improvements, but the ultimate resolution that has been achieved so far falls short of that of IN15 which uses conventional coils. Another trade-off is that conventional coils are cheaper in acquisition but more expensive in running cost (cooling water vs. liquid helium refrigeration).

The instrument will use polarized beam and will use a conventional V-cavity type transmission polarizer.

Because of the need to use long wavelength neutrons, which implies low incident flux on sample, it will be particularly important to achieve a low neutron background at the instrument. The ambient magnetic background also needs to be low, because the magnetic field integral along the beam equals the energy resolution and a relative stability/accuracy of 10^{-6} is a minimal requirement. Key parameters of NSE at HFIR are given in Table 1.

Table 1. Key parameters of a new HFIR-NSE.

Parameter	Description
Moderator or Beam Line	HFIR cold source, new CG-4 guide
Sample Size	1×1 cm^2
Beam Divergence on Sample	0.6 deg.
Sample-detector distance	4 m
Wavelength or Energy Range	8 Å $\leq \lambda \leq$ 20 Å
Resolution	τ = 500 ns, $\Delta Q/Q = 0.15$
Magnetic field integral	0.5 Tm
Detector	^{3}He 2D multiwire proportional counter, 30×30 cm^2

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